



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 AM UTC

PDB ID : 1GZX / pdb_00001gzx
Title : Oxy T State Haemoglobin - Oxygen bound at all four haems
Authors : Paoli, M.; Liddington, R.; Tame, J.; Wilkinson, A.; Dodson, G.
Deposited on : 2002-06-07
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

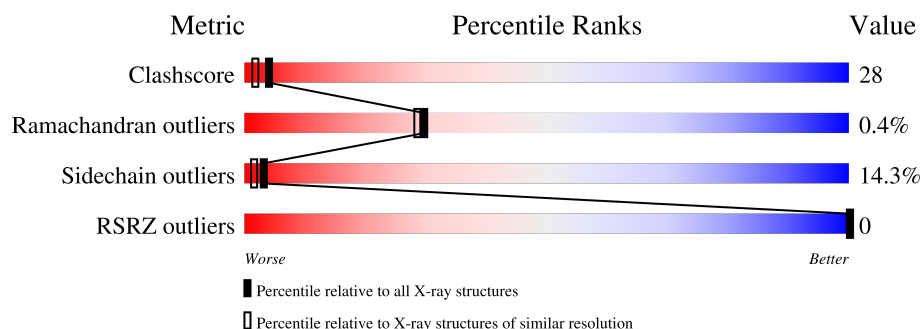
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	146	
2	D	146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OXY	B	1291	-	-	X	-
4	OXY	D	1691	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4769 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

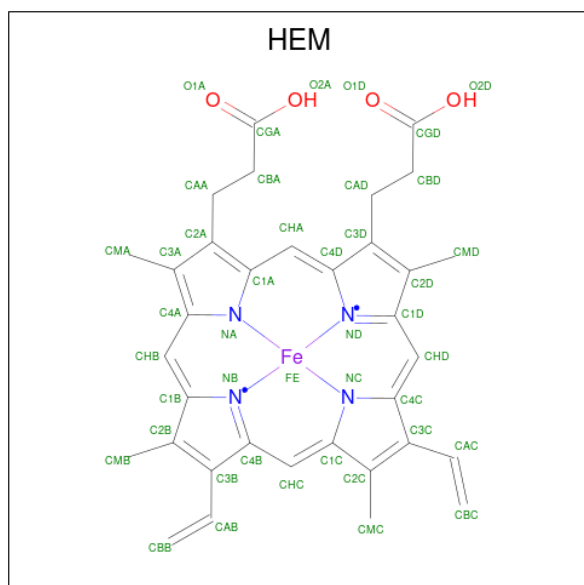
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

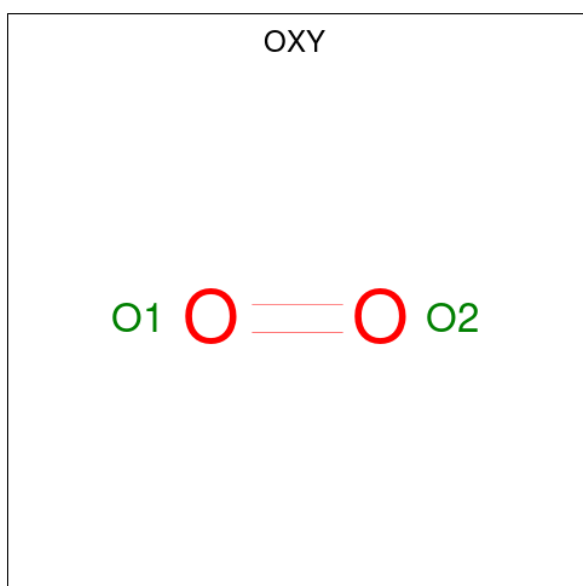
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	55	Total	O	0	0
			55	55		

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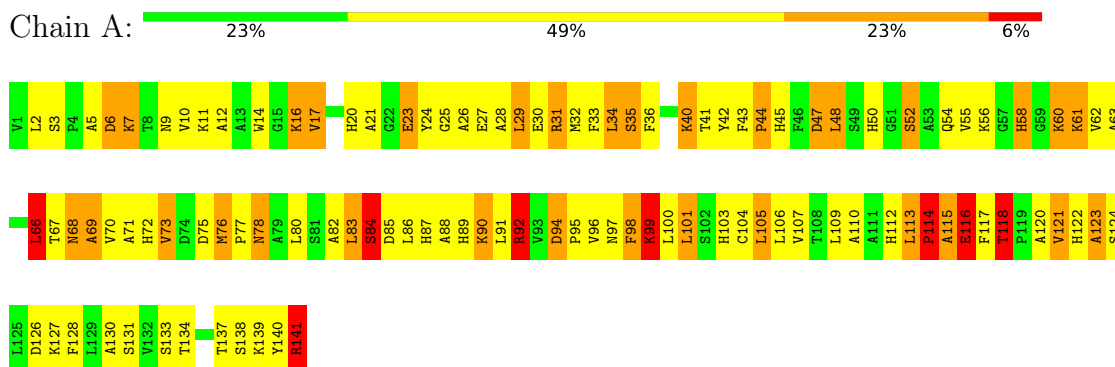
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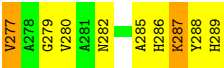
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	45	Total	O	0	0
			45	45		
5	D	43	Total	O	0	0
			43	43		

3 Residue-property plots

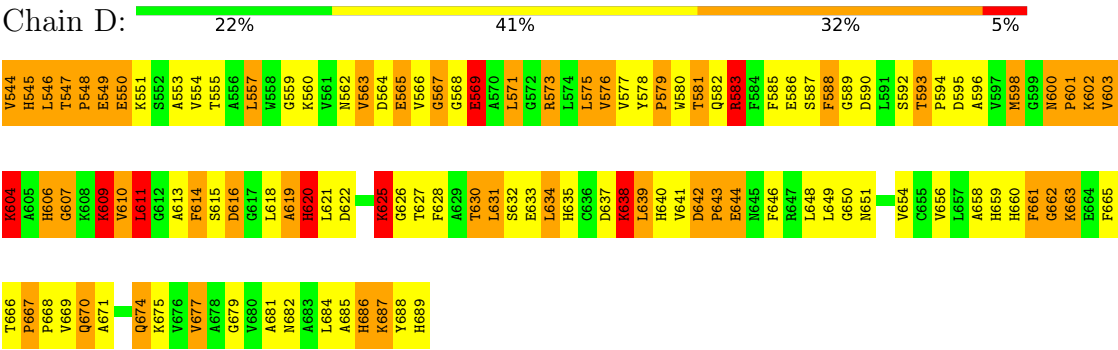
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hemoglobin subunit alpha





● Molecule 2: Hemoglobin subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.05Å 99.50Å 66.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (10.00-2.10) 93.0 (10.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.80 (at 2.10Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , 0.221 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4769	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, OXY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.49	8/1097 (0.7%)	3.34	182/1491 (12.2%)
1	C	1.50	3/1097 (0.3%)	3.16	167/1491 (11.2%)
2	B	1.47	2/1153 (0.2%)	3.34	185/1566 (11.8%)
2	D	1.44	1/1153 (0.1%)	3.30	179/1566 (11.4%)
All	All	1.47	14/4500 (0.3%)	3.29	713/6114 (11.7%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	487	HIS	CA-CB	8.96	1.67	1.53
1	A	118	THR	CA-CB	7.44	1.64	1.53
1	A	87	HIS	CA-CB	6.81	1.64	1.53
1	C	541	ARG	CD-NE	-6.42	1.37	1.46
1	A	141	ARG	NE-CZ	6.09	1.39	1.33
1	A	113	LEU	C-N	-6.08	1.26	1.34
1	A	6	ASP	C-N	5.71	1.41	1.33
1	A	67	THR	C-N	-5.64	1.26	1.34
2	B	255	CYS	N-CA	5.51	1.52	1.46
2	D	576	VAL	C-O	5.46	1.30	1.24
2	B	175	LEU	C-N	-5.42	1.27	1.33
1	A	5	ALA	N-CA	5.34	1.52	1.46
1	C	538	SER	C-O	5.22	1.30	1.24
1	A	137	THR	CA-CB	5.09	1.61	1.53

All (713) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	247	ARG	CD-NE-CZ	21.56	154.58	124.40
1	A	92	ARG	CD-NE-CZ	20.13	152.58	124.40
2	B	149	GLU	CB-CG-CD	18.87	144.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	622	ASP	CA-CB-CG	15.59	128.19	112.60
2	B	183	ARG	CD-NE-CZ	15.26	145.76	124.40
1	C	520	ALA	CA-C-O	-14.92	104.74	120.55
2	D	621	LEU	CA-C-N	13.91	141.45	120.31
2	D	621	LEU	C-N-CA	13.91	141.45	120.31
1	A	96	VAL	O-C-N	13.65	135.66	121.87
2	B	154	VAL	CA-C-O	13.11	134.75	120.85
2	B	247	ARG	NE-CZ-NH1	-13.11	108.39	121.50
1	A	112	HIS	CA-C-O	-12.75	104.88	118.90
1	C	483	LEU	CA-C-O	-12.61	107.05	120.42
2	D	620	HIS	CA-CB-CG	-12.52	101.28	113.80
2	B	183	ARG	NE-CZ-NH1	12.04	133.54	121.50
1	C	408	THR	O-C-N	11.95	136.63	122.17
2	D	588	PHE	CA-C-N	11.93	144.80	121.41
2	D	588	PHE	C-N-CA	11.93	144.80	121.41
2	D	650	GLY	O-C-N	-11.89	110.78	122.19
2	D	626	GLY	O-C-N	11.30	133.15	122.19
2	B	146	LEU	N-CA-C	-11.29	93.81	110.52
1	A	72	HIS	CA-C-O	-11.25	108.27	121.32
1	C	412	ALA	CA-C-O	-11.19	108.58	120.55
1	A	7	LYS	CG-CD-CE	11.18	137.02	111.30
2	B	222	ASP	CA-CB-CG	11.16	123.76	112.60
2	B	177	VAL	CA-C-N	11.11	136.44	123.21
2	B	177	VAL	C-N-CA	11.11	136.44	123.21
1	C	478	ASN	OD1-CG-ND2	11.11	133.71	122.60
1	A	26	ALA	CA-C-N	11.10	135.15	120.28
1	A	26	ALA	C-N-CA	11.10	135.15	120.28
2	D	626	GLY	CA-C-O	-11.02	108.98	120.66
1	C	481	SER	CA-C-O	-11.01	109.26	120.82
1	C	491	LEU	CA-C-O	-10.99	108.77	120.42
2	D	577	VAL	CA-C-N	10.95	137.47	123.34
2	D	577	VAL	C-N-CA	10.95	137.47	123.34
2	D	546	LEU	CA-C-N	10.95	138.55	121.03
2	D	546	LEU	C-N-CA	10.95	138.55	121.03
1	A	72	HIS	CA-CB-CG	-10.86	102.94	113.80
1	A	92	ARG	NE-CZ-NH2	10.79	128.91	119.20
2	B	242	ASP	CA-CB-CG	10.77	123.37	112.60
1	A	92	ARG	CA-C-N	10.73	136.47	121.66
1	A	92	ARG	C-N-CA	10.73	136.47	121.66
2	B	190	ASP	CA-CB-CG	10.69	123.29	112.60
2	B	183	ARG	NH1-CZ-NH2	-10.66	105.44	119.30
1	A	60	LYS	CA-CB-CG	10.59	135.29	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	247	ARG	NE-CZ-NH2	10.47	128.63	119.20
1	A	112	HIS	CA-CB-CG	10.41	124.21	113.80
1	A	17	VAL	N-CA-CB	10.41	122.73	110.55
1	C	443	PHE	O-C-N	10.40	130.21	121.05
1	C	432	MET	CA-C-N	10.39	134.21	120.28
1	C	432	MET	C-N-CA	10.39	134.21	120.28
2	B	216	ASP	CA-C-O	10.39	131.56	120.55
1	C	424	TYR	CA-C-O	-10.35	109.45	120.42
2	D	545	HIS	O-C-N	10.34	135.87	122.43
1	C	489	HIS	O-C-N	10.29	134.93	122.48
1	A	115	ALA	N-CA-CB	-10.22	95.03	110.16
1	A	141	ARG	CD-NE-CZ	-10.13	110.22	124.40
2	D	554	VAL	CA-C-N	10.01	133.46	120.44
2	D	554	VAL	C-N-CA	10.01	133.46	120.44
1	C	503	HIS	CA-C-N	9.98	134.66	120.28
1	C	503	HIS	C-N-CA	9.98	134.66	120.28
1	C	541	ARG	NE-CZ-NH2	9.96	128.16	119.20
1	A	96	VAL	CA-C-O	-9.96	109.92	120.57
2	B	197	VAL	CA-C-O	9.88	132.72	120.96
1	C	496	VAL	CA-C-O	-9.87	108.08	120.03
1	A	101	LEU	CA-C-O	-9.86	109.97	120.42
2	D	640	HIS	CA-CB-CG	-9.86	103.94	113.80
2	D	628	PHE	CA-C-O	-9.83	107.99	119.59
2	D	560	LYS	CA-C-N	9.82	135.55	121.80
2	D	560	LYS	C-N-CA	9.82	135.55	121.80
2	B	146	LEU	O-C-N	9.69	133.79	122.94
1	A	20	HIS	CA-CB-CG	-9.66	104.14	113.80
2	B	147	THR	N-CA-C	-9.61	97.89	110.39
2	B	208	LYS	CA-C-N	9.59	133.31	120.65
2	B	208	LYS	C-N-CA	9.59	133.31	120.65
1	C	522	HIS	CA-CB-CG	9.58	123.38	113.80
1	C	478	ASN	CA-CB-CG	-9.50	103.10	112.60
2	B	149	GLU	N-CA-C	-9.48	101.48	113.23
2	B	286	HIS	O-C-N	-9.44	112.35	122.07
2	B	169	GLU	CB-CA-C	-9.42	96.01	110.90
1	A	73	VAL	CB-CA-C	-9.42	98.30	112.05
1	A	98	PHE	O-C-N	9.40	134.92	122.33
1	A	91	LEU	CA-C-O	-9.35	111.07	120.70
1	A	69	ALA	CA-C-N	9.34	133.68	120.42
1	A	69	ALA	C-N-CA	9.34	133.68	120.42
2	D	677	VAL	CB-CA-C	9.34	124.75	112.14
2	B	228	PHE	CA-CB-CG	-9.31	104.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	607	GLY	O-C-N	-9.31	113.16	122.19
2	B	209	LYS	CA-CB-CG	9.26	132.63	114.10
2	D	677	VAL	N-CA-CB	-9.25	97.96	110.54
2	B	144	VAL	CA-C-N	-9.24	109.38	122.41
2	B	144	VAL	C-N-CA	-9.24	109.38	122.41
2	B	285	ALA	CA-C-O	9.23	130.07	119.27
2	B	222	ASP	CA-C-N	-9.20	109.14	122.67
2	B	222	ASP	C-N-CA	-9.20	109.14	122.67
2	B	149	GLU	CB-CA-C	9.17	128.17	109.55
1	C	507	VAL	O-C-N	-9.17	112.38	121.83
1	A	107	VAL	CA-C-O	-9.15	111.76	121.27
2	B	145	HIS	CA-CB-CG	-9.12	104.68	113.80
1	A	21	ALA	CA-C-N	9.07	130.05	119.98
1	A	21	ALA	C-N-CA	9.07	130.05	119.98
1	A	114	PRO	O-C-N	9.05	134.48	122.27
1	C	492	ARG	CD-NE-CZ	-9.04	111.74	124.40
2	D	686	HIS	CA-CB-CG	-8.99	104.81	113.80
2	D	658	ALA	CA-C-N	8.99	132.68	120.54
2	D	658	ALA	C-N-CA	8.99	132.68	120.54
1	A	14	TRP	CA-C-O	8.98	130.25	120.10
2	D	631	LEU	CA-C-N	8.95	132.61	120.44
2	D	631	LEU	C-N-CA	8.95	132.61	120.44
1	A	17	VAL	O-C-N	8.91	130.65	121.91
1	C	471	ALA	CA-C-O	-8.90	107.78	120.51
2	D	600	ASN	CA-C-O	8.88	127.32	119.59
1	A	104	CYS	CA-C-O	-8.87	109.77	119.97
1	C	420	HIS	CA-CB-CG	-8.86	104.94	113.80
2	B	153	ALA	CA-C-O	-8.82	111.20	120.55
2	B	229	ALA	CA-C-O	-8.77	111.26	120.55
1	A	133	SER	CA-C-O	8.75	129.83	120.55
1	C	510	ALA	CA-C-O	8.72	130.23	120.90
1	C	499	LYS	CA-C-O	-8.72	110.25	120.10
2	D	660	HIS	CA-C-O	-8.71	111.92	120.90
2	B	177	VAL	CA-C-O	-8.70	111.07	120.47
2	D	615	SER	CA-C-O	8.70	130.64	121.07
1	A	83	LEU	N-CA-C	-8.66	101.32	112.23
2	D	660	HIS	CA-CB-CG	-8.66	105.14	113.80
1	C	541	ARG	CG-CD-NE	8.63	130.99	112.00
1	C	489	HIS	CA-CB-CG	-8.62	105.18	113.80
1	A	54	GLN	O-C-N	8.59	131.37	122.09
2	D	573	ARG	NE-CZ-NH2	8.57	126.91	119.20
1	A	83	LEU	CB-CA-C	8.53	127.79	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	ASP	CA-C-O	-8.48	111.56	120.55
1	C	454	GLN	CA-C-O	-8.48	111.97	120.70
1	C	424	TYR	O-C-N	8.47	131.81	122.15
1	A	105	LEU	CA-CB-CG	8.47	145.93	116.30
1	A	83	LEU	CA-C-O	-8.45	109.82	119.79
1	C	431	ARG	NE-CZ-NH2	-8.43	111.61	119.20
1	A	3	SER	CA-C-N	8.42	128.00	119.24
1	A	3	SER	C-N-CA	8.42	128.00	119.24
1	C	513	LEU	O-C-N	8.42	129.00	121.17
1	C	472	HIS	CA-CB-CG	-8.41	105.39	113.80
2	D	660	HIS	N-CA-C	8.41	120.36	111.03
1	A	133	SER	O-C-N	-8.39	113.22	122.12
1	C	484	SER	O-C-N	8.37	133.65	122.43
1	A	91	LEU	O-C-N	8.36	131.12	122.09
1	C	540	TYR	O-C-N	8.34	131.66	122.15
2	D	553	ALA	CA-C-N	8.34	131.23	120.56
2	D	553	ALA	C-N-CA	8.34	131.23	120.56
2	B	171	LEU	CA-C-O	-8.31	112.14	120.70
2	B	190	ASP	CA-C-O	8.31	130.13	120.49
2	D	604	LYS	CB-CA-C	-8.28	97.88	110.88
2	D	637	ASP	N-CA-C	8.28	121.43	111.82
1	C	409	ASN	O-C-N	8.27	130.69	122.09
1	C	497	ASN	CA-CB-CG	-8.23	104.37	112.60
2	D	588	PHE	CA-C-O	8.22	129.50	119.31
2	B	251	ASN	CA-CB-CG	-8.21	104.39	112.60
2	D	600	ASN	CA-CB-CG	-8.20	104.40	112.60
2	D	593	THR	CA-C-O	-8.20	112.47	120.26
2	B	271	ALA	CB-CA-C	8.17	123.71	110.88
1	A	31	ARG	CD-NE-CZ	8.16	135.82	124.40
1	A	87	HIS	CA-C-O	-8.12	111.94	120.55
2	D	600	ASN	OD1-CG-ND2	8.10	130.69	122.60
2	B	237	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	29	LEU	CB-CA-C	8.07	123.66	110.90
2	D	613	ALA	N-CA-C	-8.07	102.56	111.36
2	D	659	HIS	CA-CB-CG	-8.06	105.74	113.80
2	D	598	MET	CA-C-N	8.04	130.47	120.34
2	D	598	MET	C-N-CA	8.04	130.47	120.34
1	A	5	ALA	CB-CA-C	8.03	123.48	110.88
2	D	656	VAL	CA-C-O	-8.01	112.16	121.05
1	A	120	ALA	CA-C-N	8.00	130.80	120.56
1	A	120	ALA	C-N-CA	8.00	130.80	120.56
2	B	237	ASP	CA-C-N	-7.98	108.63	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	ASP	C-N-CA	-7.98	108.63	122.36
1	C	463	ALA	CA-C-N	7.98	130.81	120.44
1	C	463	ALA	C-N-CA	7.98	130.81	120.44
1	A	100	LEU	O-C-N	7.88	131.14	122.15
2	D	640	HIS	CB-CA-C	-7.87	100.71	111.89
2	D	603	VAL	N-CA-C	-7.87	102.87	110.42
1	C	420	HIS	O-C-N	7.85	132.16	122.34
1	A	6	ASP	O-C-N	7.84	130.15	122.07
2	D	603	VAL	CA-C-O	7.83	129.47	121.17
2	D	573	ARG	NE-CZ-NH1	-7.80	113.70	121.50
2	D	638	LYS	CB-CA-C	-7.79	97.09	110.88
2	D	665	PHE	CA-CB-CG	-7.75	106.05	113.80
1	A	60	LYS	CA-C-O	7.72	128.93	120.82
2	D	643	PRO	CA-C-O	7.71	130.53	118.89
1	A	72	HIS	O-C-N	7.70	132.22	121.83
1	A	54	GLN	N-CA-CB	7.67	121.19	110.07
2	B	232	SER	O-C-N	-7.62	114.17	122.09
2	B	169	GLU	CG-CD-OE2	-7.60	100.91	118.40
1	C	486	LEU	CA-C-N	7.58	130.44	120.28
1	C	486	LEU	C-N-CA	7.58	130.44	120.28
2	D	571	LEU	N-CA-C	-7.55	102.99	111.14
2	B	150	GLU	CA-C-O	-7.52	112.51	120.55
2	B	256	VAL	CB-CA-C	7.51	122.28	112.14
2	D	610	VAL	O-C-N	-7.51	114.55	121.91
2	B	271	ALA	O-C-N	-7.48	114.36	122.07
2	B	213	ALA	N-CA-CB	7.48	120.85	110.01
1	C	502	SER	CA-C-N	7.47	130.63	120.54
1	C	502	SER	C-N-CA	7.47	130.63	120.54
1	C	473	VAL	CA-C-O	7.47	128.78	120.64
2	B	256	VAL	CA-C-O	-7.47	113.19	120.95
2	D	586	GLU	CB-CG-CD	7.46	125.29	112.60
2	B	151	LYS	N-CA-CB	7.42	121.03	110.12
1	C	517	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	48	LEU	O-C-N	7.39	131.05	122.25
1	C	514	PRO	CB-CA-C	7.37	123.71	111.56
1	C	494	ASP	CA-C-O	7.33	126.64	119.75
2	B	175	LEU	CA-C-N	7.32	129.81	120.88
2	B	175	LEU	C-N-CA	7.32	129.81	120.88
1	C	446	PHE	CA-CB-CG	7.31	121.11	113.80
1	C	420	HIS	CA-C-O	-7.31	110.80	119.35
2	B	277	VAL	N-CA-CB	-7.30	97.56	110.77
2	B	163	VAL	CA-C-O	7.29	128.37	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	550	GLU	N-CA-C	-7.29	102.32	112.45
1	A	60	LYS	CB-CG-CD	7.28	128.03	111.30
1	C	406	ASP	CA-C-O	-7.26	113.20	120.82
1	C	430	GLU	O-C-N	-7.24	114.45	122.12
2	B	191	LEU	CA-C-N	7.24	129.98	120.28
2	B	191	LEU	C-N-CA	7.24	129.98	120.28
1	A	70	VAL	CA-C-N	7.22	130.67	120.28
1	A	70	VAL	C-N-CA	7.22	130.67	120.28
1	A	123	ALA	CA-C-N	7.20	130.15	120.65
1	A	123	ALA	C-N-CA	7.20	130.15	120.65
2	D	626	GLY	N-CA-C	-7.18	103.57	112.77
1	C	478	ASN	O-C-N	7.17	130.32	122.15
1	C	458	HIS	CA-CB-CG	-7.17	106.63	113.80
2	B	255	CYS	CA-C-N	7.17	130.28	120.46
2	B	255	CYS	C-N-CA	7.17	130.28	120.46
1	C	450	HIS	CB-CA-C	-7.16	100.11	110.06
2	D	569	GLU	CA-C-O	-7.16	113.31	120.82
2	B	262	GLY	CA-C-N	7.15	130.57	120.28
2	B	262	GLY	C-N-CA	7.15	130.57	120.28
2	D	660	HIS	CG-CD2-NE2	-7.12	100.08	107.20
1	A	118	THR	CA-CB-CG2	7.11	122.59	110.50
1	A	86	LEU	CA-C-N	7.11	129.81	120.28
1	A	86	LEU	C-N-CA	7.11	129.81	120.28
2	B	146	LEU	CA-C-O	-7.09	113.36	121.72
1	A	61	LYS	CB-CG-CD	-7.08	95.01	111.30
2	B	154	VAL	CA-C-N	7.08	129.64	120.44
2	B	154	VAL	C-N-CA	7.08	129.64	120.44
2	D	662	GLY	CA-C-N	7.07	135.03	121.54
2	D	662	GLY	C-N-CA	7.07	135.03	121.54
2	D	569	GLU	CB-CA-C	-7.06	99.80	110.88
2	D	654	VAL	O-C-N	-7.05	115.03	121.87
2	D	641	VAL	CA-C-N	7.04	132.58	121.17
2	D	641	VAL	C-N-CA	7.04	132.58	121.17
1	C	517	PHE	CA-C-O	7.01	130.54	120.51
2	B	285	ALA	O-C-N	-7.01	112.85	122.46
2	B	151	LYS	CB-CA-C	-7.01	99.16	110.79
2	D	585	PHE	CA-CB-CG	-7.00	106.80	113.80
2	B	150	GLU	N-CA-CB	7.00	120.50	110.13
1	C	431	ARG	NE-CZ-NH1	7.00	128.50	121.50
2	B	173	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	C	406	ASP	O-C-N	7.00	129.28	122.07
1	A	63	ALA	CA-C-N	7.00	129.96	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ALA	C-N-CA	7.00	129.96	120.38
2	B	267	PRO	CB-CA-C	6.99	119.45	110.92
2	D	588	PHE	CA-CB-CG	-6.99	106.81	113.80
2	D	573	ARG	CA-C-O	-6.99	110.79	119.38
1	A	122	HIS	CA-C-O	-6.98	113.50	120.82
2	B	274	GLN	CA-C-N	6.97	129.50	120.44
2	B	274	GLN	C-N-CA	6.97	129.50	120.44
2	B	200	ASN	CA-CB-CG	6.96	119.56	112.60
1	C	423	GLU	OE1-CD-OE2	6.95	139.59	122.90
2	D	576	VAL	CA-CB-CG2	6.93	122.18	110.40
1	A	117	PHE	CA-C-N	6.93	135.61	121.48
1	A	117	PHE	C-N-CA	6.93	135.61	121.48
1	A	126	ASP	O-C-N	6.93	129.57	122.09
2	B	161	VAL	CA-C-O	-6.92	112.88	121.11
2	D	660	HIS	CB-CA-C	-6.92	100.23	110.95
1	A	78	ASN	CB-CG-OD1	6.91	134.62	120.80
2	D	650	GLY	CA-C-O	6.91	127.87	120.75
1	A	118	THR	CA-C-O	-6.90	113.15	120.88
2	B	155	THR	CA-CB-OG1	-6.90	99.25	109.60
1	A	122	HIS	CA-CB-CG	6.89	120.69	113.80
1	C	492	ARG	CA-C-N	6.89	130.36	120.98
1	C	492	ARG	C-N-CA	6.89	130.36	120.98
2	B	277	VAL	CB-CA-C	6.88	123.41	112.26
2	D	595	ASP	CA-C-O	-6.86	113.28	120.55
1	A	5	ALA	N-CA-CB	-6.86	100.06	110.01
1	A	131	SER	CB-CA-C	6.85	122.50	110.85
1	A	62	VAL	CA-C-N	6.84	129.78	120.54
1	A	62	VAL	C-N-CA	6.84	129.78	120.54
1	C	412	ALA	O-C-N	6.83	130.44	122.17
1	A	121	VAL	N-CA-C	-6.83	104.11	110.53
2	B	202	LYS	CA-C-O	-6.82	113.19	120.42
2	D	593	THR	O-C-N	6.82	127.92	121.71
1	C	487	HIS	N-CA-CB	6.81	120.14	110.12
2	B	193	THR	CA-C-N	6.80	126.05	118.97
2	B	193	THR	C-N-CA	6.80	126.05	118.97
1	A	30	GLU	CA-C-N	6.78	129.37	120.28
1	A	30	GLU	C-N-CA	6.78	129.37	120.28
2	D	548	PRO	N-CA-C	-6.77	105.13	114.27
1	C	499	LYS	O-C-N	6.76	130.13	122.22
2	B	216	ASP	O-C-N	-6.75	114.97	122.12
1	A	75	ASP	CA-C-O	-6.74	114.24	121.78
2	D	611	LEU	CB-CA-C	6.72	123.07	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	GLY	O-C-N	6.70	128.62	122.19
1	C	541	ARG	NE-CZ-NH1	-6.70	114.80	121.50
1	C	475	ASP	CB-CG-OD2	-6.70	103.00	118.40
2	D	642	ASP	CA-C-N	6.68	126.36	119.82
2	D	642	ASP	C-N-CA	6.68	126.36	119.82
1	A	118	THR	CA-C-N	6.67	126.45	119.05
1	A	118	THR	C-N-CA	6.67	126.45	119.05
1	C	490	LYS	CA-C-N	6.64	129.72	120.29
1	C	490	LYS	C-N-CA	6.64	129.72	120.29
2	B	155	THR	OG1-CB-CG2	6.64	122.58	109.30
1	C	481	SER	O-C-N	6.64	128.91	122.07
2	D	551	LYS	CA-C-O	-6.63	112.34	119.97
2	D	648	LEU	O-C-N	6.62	128.89	122.07
1	A	17	VAL	N-CA-C	-6.62	104.06	110.42
1	A	24	TYR	CA-C-N	6.61	127.27	119.94
1	A	24	TYR	C-N-CA	6.61	127.27	119.94
2	D	667	PRO	CB-CA-C	6.58	118.95	110.92
2	D	603	VAL	CB-CA-C	6.58	120.39	111.97
1	A	21	ALA	O-C-N	-6.56	114.56	122.11
1	C	423	GLU	CB-CG-CD	-6.55	101.46	112.60
2	D	689	HIS	CA-CB-CG	-6.54	107.26	113.80
2	B	212	GLY	O-C-N	6.54	128.53	122.19
2	D	548	PRO	CB-CA-C	6.53	120.89	111.04
2	B	207	GLY	CA-C-N	6.52	128.92	120.44
2	B	207	GLY	C-N-CA	6.52	128.92	120.44
2	B	248	LEU	O-C-N	6.51	128.78	122.07
1	C	468	ASN	N-CA-C	-6.50	104.04	112.23
2	B	267	PRO	CA-C-N	6.50	126.26	119.05
2	B	267	PRO	C-N-CA	6.50	126.26	119.05
2	B	279	GLY	CA-C-O	-6.49	113.99	121.00
2	B	222	ASP	O-C-N	6.49	131.35	122.46
1	A	103	HIS	CA-C-N	6.49	130.17	120.31
1	A	103	HIS	C-N-CA	6.49	130.17	120.31
1	C	475	ASP	CA-C-O	-6.49	113.81	122.31
2	B	287	LYS	CG-CD-CE	-6.48	96.40	111.30
1	C	525	LEU	N-CA-CB	-6.48	100.57	110.16
1	A	141	ARG	CB-CG-CD	6.48	126.19	111.30
2	B	158	TRP	CA-C-N	6.47	127.13	119.94
2	B	158	TRP	C-N-CA	6.47	127.13	119.94
2	B	210	VAL	O-C-N	-6.47	115.55	121.89
2	B	272	ALA	O-C-N	-6.45	115.28	122.12
1	C	447	ASP	N-CA-C	-6.45	98.68	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	VAL	O-C-N	6.44	128.41	121.90
1	C	498	PHE	CA-C-N	6.44	129.55	120.28
1	C	498	PHE	C-N-CA	6.44	129.55	120.28
2	D	590	ASP	O-C-N	6.44	130.66	122.93
2	D	604	LYS	N-CA-C	6.44	117.96	111.07
1	C	466	LEU	CA-C-O	6.43	127.24	120.42
1	A	128	PHE	CA-CB-CG	6.43	120.23	113.80
2	D	688	TYR	N-CA-CB	6.43	119.77	110.06
2	B	261	PHE	CA-CB-CG	-6.43	107.37	113.80
2	B	168	GLY	CA-C-N	6.42	129.18	120.44
2	B	168	GLY	C-N-CA	6.42	129.18	120.44
1	C	518	THR	CA-CB-CG2	6.41	121.40	110.50
1	C	413	ALA	CA-C-O	6.41	127.55	120.82
1	C	505	LEU	N-CA-C	-6.41	103.81	111.69
2	B	233	GLU	CB-CG-CD	6.40	123.47	112.60
1	C	498	PHE	CA-C-O	-6.39	113.77	120.55
2	D	660	HIS	ND1-CG-CD2	6.39	112.49	106.10
1	C	506	LEU	CA-C-O	-6.38	114.12	120.82
2	B	228	PHE	CA-C-O	-6.38	111.56	119.28
1	A	73	VAL	CA-CB-CG2	6.37	121.23	110.40
2	D	545	HIS	N-CA-CB	6.37	119.92	110.49
2	B	240	HIS	CA-CB-CG	-6.37	107.43	113.80
2	B	229	ALA	N-CA-C	6.36	118.22	111.28
1	C	484	SER	CA-CB-OG	-6.36	98.38	111.10
2	D	583	ARG	CD-NE-CZ	6.35	133.30	124.40
2	B	265	PHE	CA-C-N	6.35	131.86	121.57
2	B	265	PHE	C-N-CA	6.35	131.86	121.57
2	D	671	ALA	CA-C-O	-6.35	113.82	120.55
1	A	141	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	C	450	HIS	N-CA-C	6.32	119.78	110.30
1	C	405	ALA	CA-C-O	6.32	127.21	120.70
1	C	424	TYR	N-CA-C	-6.32	104.48	111.36
2	D	589	GLY	N-CA-C	6.31	128.12	113.18
1	C	435	SER	O-C-N	6.29	130.76	122.33
1	C	489	HIS	CA-C-O	-6.28	112.26	118.97
1	A	54	GLN	CA-C-O	-6.25	114.27	120.70
1	A	98	PHE	CA-C-O	-6.25	112.42	119.79
2	B	152	SER	N-CA-C	6.25	118.17	111.36
1	C	458	HIS	CA-C-N	6.24	126.91	119.98
1	C	458	HIS	C-N-CA	6.24	126.91	119.98
1	C	417	VAL	N-CA-C	-6.23	104.26	110.62
2	D	606	HIS	CA-CB-CG	-6.23	107.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	670	GLN	CA-CB-CG	-6.23	101.64	114.10
1	A	138	SER	O-C-N	6.22	129.92	122.27
2	B	239	LEU	CA-C-O	-6.21	112.34	119.60
1	A	115	ALA	CB-CA-C	6.20	121.39	110.85
1	A	60	LYS	O-C-N	-6.19	115.69	122.07
1	A	87	HIS	O-C-N	6.18	128.68	122.12
1	C	449	SER	CA-C-O	6.18	128.67	121.87
2	B	163	VAL	N-CA-C	6.17	118.76	111.05
2	B	260	HIS	CB-CA-C	-6.16	101.17	110.90
2	D	547	THR	N-CA-CB	6.15	118.91	110.05
2	D	551	LYS	N-CA-C	-6.15	104.68	111.82
2	D	654	VAL	CB-CA-C	6.14	120.43	112.14
1	C	423	GLU	CG-CD-OE2	-6.14	104.28	118.40
2	D	665	PHE	O-C-N	-6.14	115.15	122.46
1	A	126	ASP	N-CA-C	-6.14	104.51	111.14
1	A	126	ASP	CA-C-O	-6.13	114.39	120.70
2	B	282	ASN	CA-CB-CG	-6.13	106.47	112.60
1	A	25	GLY	O-C-N	-6.12	116.30	122.18
2	B	282	ASN	CA-C-O	-6.12	114.39	120.70
1	A	44	PRO	O-C-N	-6.12	114.01	122.27
2	B	155	THR	N-CA-CB	-6.11	101.14	110.01
2	B	169	GLU	OE1-CD-OE2	6.11	137.57	122.90
2	D	679	GLY	CA-C-O	6.11	127.60	121.00
1	A	61	LYS	CG-CD-CE	6.11	125.34	111.30
2	B	282	ASN	CA-C-N	6.10	128.77	120.54
2	B	282	ASN	C-N-CA	6.10	128.77	120.54
1	A	35	SER	CA-C-N	6.09	127.64	122.28
1	A	35	SER	C-N-CA	6.09	127.64	122.28
1	C	489	HIS	CA-C-N	-6.08	112.81	122.17
1	C	489	HIS	C-N-CA	-6.08	112.81	122.17
1	C	469	ALA	N-CA-C	-6.07	104.74	111.36
2	D	595	ASP	O-C-N	6.07	128.56	122.12
2	D	640	HIS	CA-C-N	6.07	130.57	122.93
2	D	640	HIS	C-N-CA	6.07	130.57	122.93
1	A	89	HIS	CA-C-N	-6.06	113.03	122.42
1	A	89	HIS	C-N-CA	-6.06	113.03	122.42
2	D	674	GLN	CG-CD-NE2	6.05	125.48	116.40
1	C	516	GLU	N-CA-C	6.05	120.39	112.89
1	A	47	ASP	O-C-N	6.04	130.08	123.13
2	D	555	THR	CB-CA-C	6.03	120.35	110.88
2	D	602	LYS	CA-CB-CG	6.02	126.14	114.10
2	B	162	ASN	OD1-CG-ND2	-6.00	116.61	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	HIS	CB-CA-C	-5.99	100.08	110.09
2	D	585	PHE	O-C-N	5.98	129.62	122.26
1	C	515	ALA	CA-C-O	-5.98	114.55	120.82
1	C	439	THR	CA-CB-OG1	-5.97	100.64	109.60
1	C	501	LEU	N-CA-CB	5.97	118.73	110.07
1	A	78	ASN	CB-CG-ND2	-5.96	107.45	116.40
2	B	260	HIS	CA-C-O	-5.96	114.56	120.70
1	A	124	SER	CA-CB-OG	-5.96	99.18	111.10
2	B	259	HIS	CA-C-N	5.95	128.53	120.44
2	B	259	HIS	C-N-CA	5.95	128.53	120.44
1	C	431	ARG	CD-NE-CZ	-5.95	116.07	124.40
1	C	500	LEU	CA-C-O	-5.95	113.64	120.24
2	B	288	TYR	CB-CG-CD1	-5.94	111.89	120.80
2	D	619	ALA	N-CA-C	-5.94	106.19	113.50
1	A	98	PHE	N-CA-C	-5.94	104.75	112.23
1	A	116	GLU	CA-CB-CG	5.94	125.97	114.10
1	A	20	HIS	ND1-CG-CD2	5.93	112.03	106.10
2	B	222	ASP	CB-CG-OD1	5.93	132.04	118.40
1	C	503	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	55	VAL	CA-C-N	5.92	128.14	120.44
1	A	55	VAL	C-N-CA	5.92	128.14	120.44
1	C	435	SER	CA-C-O	-5.92	112.80	119.79
2	B	272	ALA	CA-C-O	5.92	126.82	120.55
1	C	486	LEU	O-C-N	-5.91	115.94	122.09
2	D	658	ALA	O-C-N	-5.91	115.70	122.09
2	B	163	VAL	N-CA-CB	-5.91	100.55	110.65
2	B	230	THR	CA-C-O	-5.90	113.18	119.97
1	C	485	ASP	N-CA-C	-5.90	104.48	111.03
2	D	630	THR	CB-CA-C	5.89	120.86	110.85
2	B	150	GLU	O-C-N	5.88	129.28	122.17
2	D	625	LYS	CA-C-N	-5.87	113.54	120.00
2	D	625	LYS	C-N-CA	-5.87	113.54	120.00
1	A	103	HIS	CA-C-O	-5.87	114.66	120.82
1	A	41	THR	CA-C-N	5.87	131.98	121.66
1	A	41	THR	C-N-CA	5.87	131.98	121.66
1	C	475	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	450	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	445	HIS	CA-C-N	-5.86	112.67	122.64
1	C	445	HIS	C-N-CA	-5.86	112.67	122.64
1	A	122	HIS	CA-C-N	5.85	128.12	120.28
1	A	122	HIS	C-N-CA	5.85	128.12	120.28
1	A	118	THR	N-CA-CB	-5.85	101.71	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	567	GLY	O-C-N	5.84	128.65	122.28
2	B	222	ASP	N-CA-C	-5.84	105.99	113.23
2	B	198	MET	O-C-N	-5.84	115.39	122.22
1	C	459	GLY	O-C-N	5.83	127.79	122.19
2	B	265	PHE	CB-CA-C	5.83	121.12	112.03
1	A	41	THR	CA-CB-CG2	5.82	120.40	110.50
1	A	76	MET	CA-C-N	5.82	125.52	119.05
1	A	76	MET	C-N-CA	5.82	125.52	119.05
2	B	282	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	34	LEU	CA-C-O	-5.82	114.33	120.55
2	D	600	ASN	O-C-N	-5.82	116.93	121.47
2	B	255	CYS	CA-C-O	-5.81	114.72	120.82
2	D	551	LYS	N-CA-CB	5.81	119.29	110.28
1	A	26	ALA	O-C-N	-5.80	116.09	122.07
2	B	190	ASP	N-CA-C	5.80	118.13	109.25
2	D	555	THR	CA-C-N	5.80	127.98	120.44
2	D	555	THR	C-N-CA	5.80	127.98	120.44
1	C	415	GLY	N-CA-C	-5.79	105.66	113.24
1	C	457	GLY	N-CA-C	-5.79	105.64	112.64
2	B	277	VAL	CA-CB-CG1	5.78	120.22	110.40
2	D	639	LEU	CA-C-O	-5.77	112.31	119.18
2	D	551	LYS	CG-CD-CE	5.77	124.58	111.30
2	D	549	GLU	CB-CG-CD	5.76	122.40	112.60
2	B	172	GLY	CA-C-N	5.76	128.27	120.38
2	B	172	GLY	C-N-CA	5.76	128.27	120.38
2	B	182	GLN	OE1-CD-NE2	-5.76	116.84	122.60
2	B	226	GLY	CA-C-O	-5.76	113.93	120.09
2	B	154	VAL	O-C-N	-5.75	115.91	121.83
1	A	94	ASP	N-CA-C	-5.75	102.53	109.83
1	A	100	LEU	CA-C-O	-5.75	114.33	120.42
2	D	609	LYS	CA-C-O	5.74	126.61	120.70
2	B	274	GLN	CA-C-O	5.74	126.63	120.55
1	C	444	PRO	CA-C-N	5.74	132.76	122.38
1	C	444	PRO	C-N-CA	5.74	132.76	122.38
2	B	195	ASP	CA-CB-CG	5.73	118.33	112.60
2	D	609	LYS	O-C-N	-5.72	115.91	122.09
2	D	553	ALA	O-C-N	-5.71	115.25	122.27
1	C	494	ASP	O-C-N	-5.71	116.22	121.30
1	C	453	ALA	N-CA-CB	5.70	119.70	110.40
1	A	116	GLU	CG-CD-OE1	5.70	131.51	118.40
2	D	581	THR	CA-C-O	5.70	126.41	119.11
1	C	433	PHE	CA-CB-CG	5.70	119.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	VAL	CA-CB-CG1	5.69	120.08	110.40
2	B	226	GLY	O-C-N	5.69	128.88	122.34
1	C	421	ALA	CA-C-N	5.69	126.30	119.98
1	C	421	ALA	C-N-CA	5.69	126.30	119.98
1	A	134	THR	CA-C-O	-5.69	114.52	120.55
1	C	526	ASP	N-CA-CB	5.68	118.25	110.01
1	A	56	LYS	O-C-N	5.68	127.92	122.07
1	C	423	GLU	CB-CA-C	-5.67	99.78	110.67
2	D	644	GLU	OE1-CD-OE2	5.67	136.50	122.90
1	A	89	HIS	CA-CB-CG	-5.66	108.14	113.80
2	D	635	HIS	O-C-N	-5.66	115.70	122.15
1	A	58	HIS	CB-CA-C	5.66	121.05	110.70
2	B	286	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
2	D	640	HIS	O-C-N	-5.66	115.54	122.55
2	D	651	ASN	CA-C-O	-5.65	114.89	120.82
2	D	616	ASP	CA-C-O	-5.65	114.86	120.90
2	B	225	LYS	N-CA-C	5.64	117.11	111.07
1	A	105	LEU	N-CA-C	-5.63	104.77	111.69
1	C	406	ASP	CB-CA-C	-5.62	102.05	110.88
2	D	685	ALA	CA-C-N	5.62	128.13	120.54
2	D	685	ALA	C-N-CA	5.62	128.13	120.54
2	B	173	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
2	D	548	PRO	O-C-N	5.61	130.06	122.37
2	D	633	GLU	CB-CG-CD	-5.61	103.06	112.60
2	D	659	HIS	O-C-N	5.61	127.93	122.09
2	D	565	GLU	CB-CG-CD	5.61	122.13	112.60
2	B	147	THR	CA-C-N	5.59	125.21	119.56
2	B	147	THR	C-N-CA	5.59	125.21	119.56
2	D	622	ASP	CA-C-O	5.59	126.40	119.97
2	B	145	HIS	CA-C-O	5.59	128.45	122.13
2	D	660	HIS	CE1-NE2-CD2	5.59	114.59	109.00
1	A	40	LYS	O-C-N	5.59	129.86	122.43
2	B	169	GLU	N-CA-C	5.58	117.17	111.14
2	D	641	VAL	O-C-N	-5.58	116.84	123.03
1	A	127	LYS	CA-C-N	5.57	127.69	120.44
1	A	127	LYS	C-N-CA	5.57	127.69	120.44
1	C	409	ASN	CA-CB-CG	-5.55	107.05	112.60
2	B	161	VAL	O-C-N	5.55	129.27	122.72
2	B	285	ALA	CA-C-N	5.55	127.66	120.44
2	B	285	ALA	C-N-CA	5.55	127.66	120.44
2	D	549	GLU	CG-CD-OE1	5.55	131.17	118.40
2	B	243	PRO	O-C-N	-5.55	115.15	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	VAL	O-C-N	5.54	127.67	121.90
2	D	681	ALA	O-C-N	5.54	127.99	122.12
1	A	28	ALA	N-CA-CB	5.54	118.35	110.16
2	B	227	THR	CA-CB-CG2	5.53	119.90	110.50
1	C	497	ASN	O-C-N	5.53	129.84	122.43
1	A	68	ASN	CB-CG-OD1	-5.53	109.74	120.80
2	D	656	VAL	CB-CA-C	5.53	119.26	112.02
1	A	131	SER	O-C-N	-5.52	115.86	122.15
2	B	287	LYS	CB-CG-CD	5.52	124.00	111.30
1	A	97	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	130	ALA	O-C-N	5.52	127.75	122.07
1	A	73	VAL	O-C-N	5.52	127.47	121.90
2	B	165	GLU	CA-CB-CG	5.51	125.13	114.10
2	D	593	THR	N-CA-CB	-5.51	105.31	111.10
1	C	505	LEU	CA-C-O	-5.50	114.13	120.24
1	C	476	MET	CB-CA-C	5.50	121.00	110.17
2	D	569	GLU	CG-CD-OE2	-5.49	105.77	118.40
2	D	550	GLU	N-CA-CB	5.49	118.43	110.26
2	D	589	GLY	CA-C-N	-5.49	115.12	122.42
2	D	589	GLY	C-N-CA	-5.49	115.12	122.42
2	D	620	HIS	CB-CA-C	-5.49	102.08	111.46
2	B	270	GLN	O-C-N	5.48	128.01	122.09
2	B	157	LEU	CA-CB-CG	5.48	135.49	116.30
2	B	276	VAL	N-CA-C	5.48	116.25	110.72
1	C	506	LEU	N-CA-C	-5.47	105.21	111.07
2	D	559	GLY	CA-C-N	5.47	131.72	122.26
2	D	559	GLY	C-N-CA	5.47	131.72	122.26
1	C	510	ALA	O-C-N	-5.45	116.42	122.09
2	B	227	THR	N-CA-CB	5.44	118.05	109.94
1	C	462	VAL	CA-C-O	-5.44	115.01	121.05
1	A	54	GLN	N-CA-C	-5.43	105.28	111.14
2	B	169	GLU	CA-C-O	-5.43	115.11	120.70
1	C	481	SER	N-CA-CB	5.42	117.87	110.01
2	D	663	LYS	CA-CB-CG	5.42	124.94	114.10
1	C	446	PHE	CA-C-O	-5.41	114.89	121.28
2	D	661	PHE	O-C-N	5.41	129.84	122.37
2	B	161	VAL	CA-C-N	-5.40	114.47	122.41
2	B	161	VAL	C-N-CA	-5.40	114.47	122.41
2	D	614	PHE	CB-CA-C	5.40	119.35	110.88
2	D	587	SER	CA-CB-OG	5.39	121.89	111.10
1	C	432	MET	O-C-N	-5.39	116.27	122.09
2	B	191	LEU	N-CA-CB	-5.39	102.09	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	GLY	CA-C-O	-5.39	115.18	121.00
1	C	478	ASN	CB-CG-ND2	-5.38	108.33	116.40
1	A	116	GLU	CA-C-O	-5.38	113.23	119.14
1	A	84	SER	N-CA-CB	5.37	118.01	110.12
1	C	492	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	C	527	LYS	CA-C-N	5.36	127.41	120.44
1	C	527	LYS	C-N-CA	5.36	127.41	120.44
1	A	20	HIS	CG-CD2-NE2	-5.36	101.84	107.20
1	A	56	LYS	N-CA-C	-5.36	105.33	111.07
2	D	679	GLY	O-C-N	-5.36	117.03	122.18
1	A	9	ASN	O-C-N	5.35	128.25	122.15
2	B	245	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	101	LEU	N-CA-C	-5.35	105.53	111.36
2	B	153	ALA	O-C-N	5.35	127.79	122.12
2	D	642	ASP	CB-CA-C	5.34	118.64	109.82
1	A	133	SER	CA-C-N	5.34	127.43	120.28
1	A	133	SER	C-N-CA	5.34	127.43	120.28
2	D	571	LEU	CA-C-O	-5.34	115.20	120.70
2	D	579	PRO	CA-C-N	-5.32	111.30	121.94
2	D	579	PRO	C-N-CA	-5.32	111.30	121.94
1	A	99	LYS	N-CA-CB	5.32	118.03	110.16
2	D	596	ALA	N-CA-C	-5.32	105.38	111.07
2	B	209	LYS	N-CA-CB	5.32	117.67	109.91
1	A	23	GLU	O-C-N	-5.31	116.09	122.15
2	B	174	LEU	CA-C-N	5.31	127.93	120.28
2	B	174	LEU	C-N-CA	5.31	127.93	120.28
1	C	406	ASP	OD1-CG-OD2	5.31	135.64	122.90
2	D	555	THR	CA-C-O	-5.31	115.25	120.82
1	A	114	PRO	CA-CB-CG	-5.31	94.42	104.50
2	B	247	ARG	CA-C-O	-5.31	114.80	120.42
1	C	433	PHE	O-C-N	5.30	127.74	122.12
1	A	127	LYS	CA-C-O	-5.29	114.94	120.55
1	C	453	ALA	N-CA-C	-5.29	106.33	112.89
2	D	632	SER	CA-C-O	5.27	126.12	120.70
1	A	87	HIS	N-CA-CB	5.26	117.86	110.12
2	B	286	HIS	N-CA-C	5.26	116.70	111.07
1	C	466	LEU	N-CA-CB	-5.25	102.39	110.16
2	D	686	HIS	N-CA-C	5.25	117.41	111.11
2	D	602	LYS	N-CA-CB	5.25	118.02	110.20
1	C	478	ASN	CA-C-O	-5.25	114.86	120.42
1	A	82	ALA	O-C-N	5.24	128.13	122.15
1	C	409	ASN	CB-CG-ND2	5.24	124.27	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASN	N-CA-C	-5.24	105.01	111.40
2	D	601	PRO	CB-CA-C	5.24	118.94	111.04
2	D	564	ASP	O-C-N	5.23	127.47	122.03
2	B	286	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	25	GLY	N-CA-C	-5.23	106.44	112.50
1	A	110	ALA	CA-C-O	-5.22	115.01	120.55
1	A	116	GLU	N-CA-CB	5.22	118.21	110.53
1	A	140	TYR	N-CA-C	5.22	118.11	111.69
1	C	429	LEU	CA-C-N	5.22	127.53	120.38
1	C	429	LEU	C-N-CA	5.22	127.53	120.38
2	B	286	HIS	CA-C-N	5.21	131.53	122.56
2	B	286	HIS	C-N-CA	5.21	131.53	122.56
2	D	566	VAL	CB-CA-C	5.21	119.42	112.22
1	A	31	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	C	475	ASP	O-C-N	5.21	132.54	121.35
2	D	568	GLY	N-CA-C	-5.21	106.19	112.49
1	C	441	THR	CA-CB-OG1	-5.20	101.80	109.60
1	C	468	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	C	501	LEU	CB-CA-C	-5.18	102.71	110.90
1	C	511	ALA	O-C-N	5.18	129.37	122.43
2	D	625	LYS	CB-CA-C	-5.17	102.20	110.79
1	C	509	LEU	CA-C-N	5.17	127.52	120.54
1	C	509	LEU	C-N-CA	5.17	127.52	120.54
1	A	66	LEU	CA-C-O	5.17	126.25	120.82
1	A	71	ALA	O-C-N	-5.17	116.17	122.22
2	B	148	PRO	CA-C-N	-5.17	112.57	121.66
2	B	148	PRO	C-N-CA	-5.17	112.57	121.66
2	B	160	LYS	O-C-N	-5.17	115.24	122.37
1	A	104	CYS	CA-C-N	5.16	129.40	120.58
1	A	104	CYS	C-N-CA	5.16	129.40	120.58
1	A	12	ALA	CA-C-O	-5.15	114.96	120.42
1	C	539	LYS	N-CA-CB	-5.15	102.72	111.17
1	C	468	ASN	CB-CA-C	5.15	120.88	110.38
1	C	492	ARG	N-CA-C	5.15	118.54	111.54
1	A	47	ASP	CA-CB-CG	-5.14	107.45	112.60
2	B	196	ALA	N-CA-C	-5.14	105.67	111.28
2	B	171	LEU	N-CA-CB	5.14	117.52	110.07
1	C	530	ALA	O-C-N	-5.14	116.67	122.12
1	A	14	TRP	O-C-N	-5.14	116.21	122.22
1	A	121	VAL	CA-CB-CG1	5.14	119.13	110.40
2	B	286	HIS	CB-CA-C	5.14	118.94	110.88
1	C	508	THR	CA-C-N	5.13	127.11	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	508	THR	C-N-CA	5.13	127.11	120.44
2	B	215	SER	CA-CB-OG	-5.13	100.84	111.10
1	A	84	SER	CB-CA-C	-5.13	102.28	110.79
1	C	472	HIS	CB-CA-C	-5.12	100.55	110.75
2	B	146	LEU	N-CA-CB	5.12	118.65	110.46
2	B	260	HIS	CA-CB-CG	5.12	118.92	113.80
2	D	578	TYR	CA-CB-CG	-5.12	104.69	113.90
2	B	175	LEU	CA-C-O	-5.11	114.33	120.10
2	D	586	GLU	O-C-N	5.11	127.98	122.11
2	B	231	LEU	N-CA-C	-5.11	105.79	111.36
2	B	191	LEU	CA-C-O	5.10	125.50	119.48
2	D	622	ASP	CB-CG-OD1	5.10	130.13	118.40
1	A	50	HIS	CA-C-O	5.10	126.73	120.92
1	C	512	HIS	CA-CB-CG	5.09	118.89	113.80
2	D	578	TYR	CA-C-N	5.08	126.20	119.84
2	D	578	TYR	C-N-CA	5.08	126.20	119.84
2	B	226	GLY	N-CA-C	-5.08	106.23	113.86
1	C	489	HIS	N-CA-C	5.08	120.48	113.97
1	A	36	PHE	CA-C-N	5.08	124.80	119.82
1	A	36	PHE	C-N-CA	5.08	124.80	119.82
2	D	547	THR	N-CA-C	-5.08	102.89	110.20
1	C	428	ALA	CA-C-O	-5.07	115.17	120.55
2	D	634	LEU	N-CA-CB	-5.07	102.66	110.16
2	D	651	ASN	CB-CG-ND2	-5.07	108.80	116.40
1	A	44	PRO	CA-C-O	5.05	126.77	119.34
1	C	504	CYS	CA-CB-SG	-5.05	102.79	114.40
1	A	76	MET	O-C-N	5.04	125.44	120.71
2	D	620	HIS	N-CA-C	5.03	118.49	111.30
1	A	72	HIS	CB-CA-C	-5.03	102.80	111.45
1	A	25	GLY	CA-C-N	5.03	126.97	120.44
1	A	25	GLY	C-N-CA	5.03	126.97	120.44
2	D	682	ASN	O-C-N	5.03	127.88	122.15
1	C	490	LYS	CA-C-O	-5.02	113.38	119.61
1	C	487	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	24	TYR	CA-CB-CG	5.01	122.92	113.90
2	B	195	ASP	O-C-N	5.01	127.43	122.12
1	A	68	ASN	O-C-N	-5.00	116.12	122.27
2	D	638	LYS	CA-CB-CG	-5.00	104.09	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	49	0
1	C	1069	0	1070	54	0
2	B	1123	0	1115	52	0
2	D	1123	0	1115	111	0
3	A	43	0	30	3	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	10	0
4	A	2	0	0	0	0
4	B	2	0	0	2	0
4	C	2	0	0	0	0
4	D	2	0	0	2	0
5	A	62	0	0	4	0
5	B	55	0	0	7	0
5	C	45	0	0	2	1
5	D	43	0	0	8	0
All	All	4769	0	4493	251	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:638:LYS:HB2	2:D:638:LYS:NZ	1.27	1.29
1:C:470:VAL:O	1:C:473:VAL:HG22	1.39	1.18
2:D:547:THR:HG22	2:D:549:GLU:N	1.64	1.13
2:D:649:LEU:HD23	3:D:1690:HEM:HBB2	1.32	1.09
2:D:638:LYS:NZ	2:D:638:LYS:CB	2.17	1.07
2:D:544:VAL:HG13	2:D:546:LEU:HD13	1.36	1.07
2:D:547:THR:HG22	2:D:549:GLU:H	0.82	0.97
2:B:144:VAL:HG22	2:B:145:HIS:H	1.31	0.96
2:D:620:HIS:HB2	5:D:2022:HOH:O	1.65	0.95
1:C:470:VAL:O	1:C:473:VAL:CG2	2.15	0.94
2:D:547:THR:CG2	2:D:549:GLU:H	1.78	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:563:VAL:HG22	2:D:611:LEU:HD12	1.51	0.93
1:A:16:LYS:NZ	1:A:16:LYS:HB3	1.84	0.91
2:D:638:LYS:CB	2:D:638:LYS:HZ2	1.78	0.91
2:D:620:HIS:N	2:D:620:HIS:CD2	2.36	0.90
2:D:627:THR:CB	5:D:2022:HOH:O	2.20	0.89
2:D:610:VAL:HG21	4:D:1691:OXY:O1	1.73	0.89
1:C:513:LEU:HB3	1:C:516:GLU:HG2	1.53	0.88
2:D:638:LYS:HB2	2:D:638:LYS:HZ3	1.39	0.88
2:D:544:VAL:CG1	2:D:546:LEU:HD13	2.05	0.87
2:D:547:THR:HG21	2:D:549:GLU:HB2	1.57	0.84
1:C:512:HIS:C	1:C:514:PRO:HD3	2.03	0.83
2:D:627:THR:OG1	5:D:2022:HOH:O	1.94	0.82
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.60	0.81
2:D:620:HIS:N	2:D:620:HIS:HD2	1.76	0.80
2:D:544:VAL:HG13	2:D:546:LEU:CD1	2.10	0.80
2:B:144:VAL:HG22	2:B:145:HIS:N	1.95	0.80
2:D:667:PRO:N	2:D:668:PRO:CD	2.45	0.80
1:C:439:THR:HG22	1:C:497:ASN:HD22	1.48	0.79
2:B:267:PRO:HD2	2:B:268:PRO:HD3	1.63	0.79
1:C:518:THR:HG23	1:C:521:VAL:H	1.48	0.79
1:A:35:SER:HB3	2:B:274:GLN:HG3	1.64	0.78
2:D:638:LYS:HA	2:D:638:LYS:HE3	1.62	0.78
2:B:180:TRP:HZ3	1:C:541:ARG:HG2	1.50	0.76
2:D:634:LEU:HD12	2:D:638:LYS:HZ3	1.52	0.75
1:C:443:PHE:N	1:C:444:PRO:CD	2.50	0.74
1:A:114:PRO:O	2:B:259:HIS:NE2	2.20	0.74
2:B:267:PRO:CD	2:B:268:PRO:HD3	2.18	0.74
2:B:144:VAL:CG2	2:B:145:HIS:H	2.01	0.74
1:A:99:LYS:HD2	1:A:99:LYS:N	2.03	0.74
2:D:649:LEU:CD2	3:D:1690:HEM:HBB2	2.13	0.74
2:D:619:ALA:C	2:D:620:HIS:CD2	2.66	0.73
2:D:619:ALA:C	2:D:620:HIS:HD2	1.96	0.73
2:D:563:VAL:HG22	2:D:611:LEU:CD1	2.17	0.73
2:D:638:LYS:HE3	2:D:638:LYS:CA	2.17	0.73
2:D:547:THR:CG2	2:D:549:GLU:HB2	2.17	0.73
1:A:92:ARG:HB3	2:D:580:TRP:HB2	1.71	0.73
1:C:485:ASP:OD1	1:C:539:LYS:HE2	1.88	0.72
2:D:634:LEU:O	2:D:638:LYS:HB3	1.90	0.71
2:D:667:PRO:N	2:D:668:PRO:HD2	2.04	0.71
2:D:638:LYS:HB2	2:D:638:LYS:HZ2	0.89	0.71
2:B:186:GLU:HG2	5:B:2012:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:MET:N	1:C:477:PRO:CD	2.54	0.70
1:A:99:LYS:HD2	1:A:99:LYS:H	1.56	0.70
1:C:428:ALA:CB	1:C:505:LEU:HD13	2.22	0.69
2:D:600:ASN:OD1	2:D:602:LYS:N	2.22	0.69
2:B:164:ASP:CG	2:B:208:LYS:HD2	2.17	0.69
2:D:687:LYS:HD2	5:D:2040:HOH:O	1.94	0.68
2:B:164:ASP:OD2	2:B:208:LYS:HD2	1.95	0.67
2:B:267:PRO:N	2:B:268:PRO:CD	2.58	0.67
1:A:90:LYS:HB2	1:A:90:LYS:NZ	2.10	0.66
1:A:114:PRO:HG2	1:A:115:ALA:N	2.09	0.66
2:D:667:PRO:CD	2:D:668:PRO:CD	2.73	0.66
1:A:16:LYS:HB3	1:A:16:LYS:HZ3	1.60	0.65
1:A:90:LYS:HB2	1:A:90:LYS:HZ2	1.60	0.65
2:B:209:LYS:HE2	5:B:2054:HOH:O	1.97	0.65
2:D:610:VAL:CG2	4:D:1691:OXY:O1	2.44	0.64
2:B:237:ASP:OD2	2:B:289:HIS:NE2	2.30	0.64
1:C:513:LEU:N	1:C:514:PRO:HD3	2.13	0.64
1:C:518:THR:CG2	1:C:521:VAL:HG23	2.27	0.64
1:C:428:ALA:HB2	1:C:505:LEU:HD13	1.79	0.64
2:D:614:PHE:CE1	5:D:2005:HOH:O	2.50	0.64
2:D:609:LYS:HD3	3:D:1690:HEM:HAA2	1.79	0.63
1:C:468:ASN:O	1:C:472:HIS:HD2	1.80	0.63
2:D:569:GLU:O	2:D:573:ARG:HG3	1.98	0.63
2:D:634:LEU:HD12	2:D:638:LYS:NZ	2.13	0.63
2:D:667:PRO:HD2	2:D:668:PRO:CD	2.28	0.63
1:C:518:THR:HG22	1:C:521:VAL:CG2	2.29	0.62
2:B:144:VAL:HG13	2:B:146:LEU:HD23	1.82	0.62
2:B:229:ALA:O	2:B:233:GLU:HG3	2.00	0.61
2:D:667:PRO:CD	2:D:668:PRO:HD3	2.29	0.61
1:A:92:ARG:HB2	2:D:583:ARG:HD3	1.82	0.61
2:D:594:PRO:O	2:D:598:MET:HG2	2.00	0.61
2:B:150:GLU:OE2	2:B:275:LYS:NZ	2.33	0.61
2:B:151:LYS:O	2:B:155:THR:HB	2.01	0.60
2:D:625:LYS:HD3	2:D:686:HIS:CG	2.36	0.60
2:D:638:LYS:CA	2:D:638:LYS:CE	2.76	0.60
1:C:443:PHE:N	1:C:444:PRO:HD3	2.17	0.59
1:A:85:ASP:OD1	1:A:139:LYS:HD3	2.03	0.59
1:C:484:SER:HB2	5:C:2029:HOH:O	2.03	0.59
2:B:146:LEU:HD13	2:B:150:GLU:HB3	1.85	0.59
2:B:276:VAL:O	2:B:280:VAL:HG23	2.03	0.59
1:C:501:LEU:HD22	1:C:505:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:667:PRO:HD2	2:D:668:PRO:HD3	1.84	0.59
2:B:287:LYS:HE2	5:B:2052:HOH:O	2.02	0.58
2:D:627:THR:HB	5:D:2022:HOH:O	1.94	0.58
1:A:6:ASP:O	1:A:10:VAL:HG23	2.03	0.58
2:D:592:SER:C	2:D:593:THR:HG23	2.28	0.58
1:A:114:PRO:HA	2:B:259:HIS:CD2	2.38	0.58
2:B:144:VAL:HG21	5:B:2047:HOH:O	2.04	0.58
1:C:439:THR:HG22	1:C:497:ASN:ND2	2.17	0.58
2:D:547:THR:CG2	2:D:548:PRO:CD	2.82	0.57
1:C:518:THR:HG22	1:C:521:VAL:HB	1.85	0.57
2:D:547:THR:HG23	2:D:548:PRO:CD	2.33	0.57
2:D:588:PHE:HD2	2:D:588:PHE:N	2.02	0.57
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.40	0.56
2:D:576:VAL:HG22	2:D:594:PRO:HA	1.87	0.56
2:D:588:PHE:N	2:D:588:PHE:CD2	2.72	0.56
2:D:625:LYS:HE3	2:D:686:HIS:CD2	2.40	0.56
1:A:114:PRO:HG2	1:A:115:ALA:H	1.71	0.56
2:D:667:PRO:CD	2:D:668:PRO:HD2	2.35	0.55
1:A:123:ALA:HB1	5:A:2054:HOH:O	2.06	0.55
2:D:544:VAL:HG23	5:D:2035:HOH:O	2.06	0.55
2:D:571:LEU:HD21	2:D:606:HIS:HD2	1.72	0.55
1:A:114:PRO:HA	2:B:259:HIS:NE2	2.23	0.54
5:A:2050:HOH:O	2:B:263:LYS:HD2	2.07	0.54
1:C:440:LYS:HG2	1:C:448:LEU:HD13	1.90	0.54
1:C:518:THR:HG22	1:C:521:VAL:HG23	1.88	0.54
2:B:147:THR:O	2:B:150:GLU:HB2	2.07	0.54
2:B:169:GLU:HG2	2:B:256:VAL:HG13	1.89	0.54
1:C:424:TYR:N	1:C:424:TYR:CD2	2.75	0.54
2:D:609:LYS:HD3	3:D:1690:HEM:CAA	2.37	0.54
2:D:639:LEU:HD13	3:D:1690:HEM:C3D	2.42	0.53
2:B:267:PRO:CD	2:B:268:PRO:CD	2.86	0.53
2:D:547:THR:HG23	2:D:548:PRO:HD2	1.90	0.53
2:B:267:PRO:HD2	2:B:268:PRO:CD	2.34	0.53
2:B:202:LYS:HG3	5:B:2020:HOH:O	2.09	0.53
3:B:1290:HEM:HBC2	3:B:1290:HEM:HMC2	1.92	0.52
1:A:118:THR:HG23	5:A:2051:HOH:O	2.09	0.52
1:C:488:ALA:HA	1:C:540:TYR:CE2	2.45	0.52
2:B:186:GLU:HG3	5:B:2014:HOH:O	2.08	0.52
2:D:571:LEU:CD2	2:D:606:HIS:HD2	2.23	0.52
1:C:442:TYR:C	1:C:444:PRO:CD	2.82	0.51
2:D:600:ASN:OD1	2:D:600:ASN:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:661:PHE:O	2:D:662:GLY:C	2.53	0.51
1:A:141:ARG:HD3	1:C:527:LYS:HG2	1.93	0.51
2:D:547:THR:HB	2:D:550:GLU:HG3	1.91	0.51
2:D:576:VAL:CG2	2:D:594:PRO:HA	2.40	0.51
2:D:667:PRO:HD2	2:D:668:PRO:HD2	1.92	0.51
1:C:518:THR:HG22	1:C:521:VAL:CB	2.40	0.51
2:B:144:VAL:CG2	2:B:145:HIS:N	2.62	0.51
2:D:666:THR:C	2:D:668:PRO:HD2	2.36	0.50
2:B:235:HIS:HA	2:B:239:LEU:HB2	1.94	0.50
2:B:267:PRO:CB	2:B:268:PRO:HD3	2.42	0.50
1:C:513:LEU:N	1:C:514:PRO:CD	2.74	0.50
2:B:147:THR:HG23	2:B:148:PRO:HD2	1.93	0.50
2:D:643:PRO:HA	2:D:646:PHE:CD2	2.46	0.50
2:D:592:SER:O	2:D:593:THR:CG2	2.60	0.50
2:B:210:VAL:HG21	4:B:1291:OXY:O1	2.12	0.50
1:A:43:PHE:N	1:A:44:PRO:CD	2.75	0.49
1:A:47:ASP:OD2	1:A:52:SER:HB2	2.12	0.49
1:C:516:GLU:H	1:C:516:GLU:CD	2.19	0.49
2:D:563:VAL:CG2	2:D:611:LEU:HD12	2.32	0.49
2:D:666:THR:OG1	2:D:669:VAL:HG23	2.13	0.49
1:C:476:MET:N	1:C:477:PRO:HD2	2.28	0.49
2:D:598:MET:O	2:D:604:LYS:NZ	2.37	0.49
2:B:287:LYS:CE	5:B:2052:HOH:O	2.61	0.49
2:B:267:PRO:HB2	2:B:268:PRO:HD3	1.95	0.48
1:C:442:TYR:C	1:C:444:PRO:HD2	2.38	0.48
2:D:634:LEU:CD1	2:D:638:LYS:HZ3	2.24	0.48
1:C:440:LYS:HG2	1:C:448:LEU:CD1	2.43	0.48
1:A:113:LEU:HB3	1:A:116:GLU:HG2	1.96	0.48
2:B:146:LEU:CD1	2:B:150:GLU:HB3	2.44	0.48
2:D:684:LEU:CD1	3:D:1690:HEM:HAB	2.43	0.48
1:A:7:LYS:O	1:A:11:LYS:HG2	2.13	0.48
1:C:431:ARG:HD3	2:D:670:GLN:OE1	2.14	0.48
1:A:92:ARG:HB2	2:D:583:ARG:CD	2.44	0.47
2:D:567:GLY:O	2:D:607:GLY:HA3	2.14	0.47
3:D:1690:HEM:HBA2	3:D:1690:HEM:HHA	1.96	0.47
1:C:442:TYR:CE1	1:C:493:VAL:HA	2.50	0.47
2:D:592:SER:O	2:D:593:THR:HG23	2.15	0.47
1:C:484:SER:O	1:C:488:ALA:CB	2.63	0.47
1:A:114:PRO:HA	2:B:259:HIS:HE2	1.80	0.47
1:A:88:ALA:HB2	5:A:2061:HOH:O	2.15	0.46
1:A:114:PRO:C	2:B:259:HIS:HE2	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:CG	1:A:115:ALA:N	2.78	0.46
2:D:592:SER:C	2:D:593:THR:CG2	2.89	0.46
1:A:83:LEU:HD11	3:A:1142:HEM:C3A	2.51	0.46
2:B:157:LEU:C	2:B:159:GLY:N	2.71	0.46
2:B:243:PRO:HG2	1:C:438:THR:CG2	2.45	0.46
2:D:575:LEU:HG	2:D:582:GLN:HG2	1.96	0.46
2:B:200:ASN:OD1	2:B:202:LYS:HB2	2.16	0.45
1:A:29:LEU:HD11	1:A:58:HIS:HD2	1.80	0.45
2:D:544:VAL:CG1	2:D:546:LEU:CD1	2.83	0.45
1:C:506:LEU:HD12	1:C:506:LEU:HA	1.73	0.45
2:D:631:LEU:HD23	2:D:631:LEU:HA	1.74	0.45
1:C:482:ALA:O	1:C:485:ASP:HB2	2.17	0.45
1:A:84:SER:CB	1:A:139:LYS:HD2	2.42	0.45
2:D:634:LEU:O	2:D:638:LYS:CB	2.63	0.45
2:B:243:PRO:HG2	1:C:438:THR:HG22	1.98	0.44
2:D:547:THR:HG22	2:D:549:GLU:CA	2.43	0.44
1:A:27:GLU:O	1:A:31:ARG:HG3	2.17	0.44
1:C:418:GLY:O	1:C:420:HIS:N	2.51	0.44
2:D:649:LEU:HD22	3:D:1690:HEM:HMC3	1.99	0.44
1:C:516:GLU:CD	1:C:516:GLU:N	2.76	0.44
2:D:642:ASP:C	2:D:644:GLU:H	2.26	0.44
2:D:547:THR:CG2	2:D:548:PRO:HD2	2.48	0.44
1:C:402:LEU:HD12	1:C:402:LEU:HA	1.83	0.44
1:A:66:LEU:HD21	1:A:105:LEU:HD21	1.99	0.43
1:C:427:GLU:O	1:C:431:ARG:HG3	2.17	0.43
2:D:642:ASP:C	2:D:644:GLU:N	2.76	0.43
1:C:466:LEU:O	1:C:470:VAL:HG23	2.19	0.43
2:D:547:THR:CG2	2:D:549:GLU:CB	2.94	0.43
2:D:667:PRO:CB	2:D:668:PRO:HD3	2.48	0.43
1:A:78:ASN:HD22	1:A:78:ASN:HA	1.58	0.43
2:D:579:PRO:O	2:D:582:GLN:HG3	2.19	0.43
1:A:43:PHE:N	1:A:43:PHE:CD1	2.87	0.43
2:B:178:TYR:N	2:B:179:PRO:CD	2.80	0.43
1:C:451:GLY:O	1:C:452:SER:C	2.62	0.43
2:D:557:LEU:C	2:D:557:LEU:HD13	2.44	0.43
2:D:625:LYS:NZ	5:D:2020:HOH:O	2.52	0.43
1:A:76:MET:N	1:A:77:PRO:CD	2.81	0.43
1:A:16:LYS:HB3	1:A:16:LYS:HZ2	1.76	0.43
1:A:61:LYS:HD3	3:A:1142:HEM:HAA2	2.01	0.42
1:C:472:HIS:C	1:C:474:ASP:N	2.77	0.42
1:C:494:ASP:O	1:C:495:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:575:LEU:HD12	2:D:581:THR:OG1	2.19	0.42
2:D:666:THR:HB	2:D:668:PRO:HD2	2.02	0.42
2:B:157:LEU:C	2:B:159:GLY:H	2.25	0.42
2:D:545:HIS:O	2:D:675:LYS:HE2	2.19	0.42
2:D:547:THR:CG2	2:D:548:PRO:N	2.82	0.42
2:D:562:ASN:CG	2:D:565:GLU:HG3	2.43	0.42
2:D:625:LYS:HD3	2:D:686:HIS:CD2	2.54	0.42
1:A:98:PHE:HD1	3:A:1142:HEM:HBB2	1.85	0.42
2:D:611:LEU:HD22	2:D:611:LEU:HA	1.68	0.42
2:D:642:ASP:HA	2:D:643:PRO:HD3	1.82	0.42
1:C:444:PRO:HG2	5:C:2017:HOH:O	2.18	0.42
1:A:42:TYR:C	1:A:44:PRO:CD	2.92	0.42
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.85	0.42
1:C:435:SER:HB3	2:D:674:GLN:HG3	2.01	0.42
2:D:571:LEU:HD12	2:D:571:LEU:HA	1.71	0.42
1:C:424:TYR:N	1:C:424:TYR:HD2	2.15	0.41
2:D:634:LEU:HD12	2:D:638:LYS:HB2	2.02	0.41
1:A:69:ALA:HB2	1:A:80:LEU:HD21	2.02	0.41
2:D:616:ASP:O	2:D:620:HIS:CD2	2.72	0.41
2:B:175:LEU:HG	2:B:182:GLN:HG2	2.01	0.41
1:C:484:SER:O	1:C:488:ALA:HB3	2.20	0.41
2:D:547:THR:HG22	2:D:548:PRO:N	2.31	0.41
1:A:33:PHE:CD1	1:A:40:LYS:HG2	2.55	0.41
2:B:232:SER:HB3	2:B:287:LYS:HG2	2.02	0.41
1:A:118:THR:HG22	1:A:121:VAL:H	1.86	0.41
1:A:34:LEU:HD12	2:B:267:PRO:HB2	2.03	0.41
1:A:85:ASP:CG	1:A:139:LYS:HZ3	2.29	0.41
2:D:609:LYS:HE2	3:D:1690:HEM:O1A	2.20	0.41
2:B:206:HIS:NE2	4:B:1291:OXY:O1	2.53	0.40
1:C:472:HIS:C	1:C:474:ASP:H	2.28	0.40
2:D:643:PRO:HA	2:D:646:PHE:CE2	2.56	0.40
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.55	0.40
2:B:148:PRO:HA	2:B:151:LYS:HG3	2.02	0.40
1:C:431:ARG:HA	2:D:667:PRO:HB3	2.03	0.40
2:D:639:LEU:HD13	3:D:1690:HEM:C2D	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2027:HOH:O	5:C:2027:HOH:O[2_565]	1.90	0.30

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	15
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	18	15
All	All	566/574 (99%)	543 (96%)	21 (4%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	419	ALA
2	D	663	LYS

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	92 (81%)	21 (19%)	1	1
1	C	113/113 (100%)	99 (88%)	14 (12%)	4	2
2	B	118/118 (100%)	105 (89%)	13 (11%)	6	3
2	D	118/118 (100%)	100 (85%)	18 (15%)	3	1
All	All	462/462 (100%)	396 (86%)	66 (14%)	3	1

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	16	LYS
1	A	17	VAL
1	A	23	GLU
1	A	32	MET
1	A	52	SER
1	A	60	LYS
1	A	66	LEU
1	A	68	ASN
1	A	73	VAL
1	A	84	SER
1	A	90	LYS
1	A	92	ARG
1	A	99	LYS
1	A	101	LEU
1	A	106	LEU
1	A	109	LEU
1	A	114	PRO
1	A	116	GLU
1	A	118	THR
1	A	141	ARG
2	B	146	LEU
2	B	147	THR
2	B	149	GLU
2	B	155	THR
2	B	157	LEU
2	B	160	LYS
2	B	163	VAL
2	B	164	ASP
2	B	204	LYS
2	B	211	LEU
2	B	215	SER
2	B	238	LYS
2	B	277	VAL
1	C	402	LEU
1	C	416	LYS
1	C	417	VAL
1	C	456	LYS
1	C	473	VAL
1	C	481	SER
1	C	484	SER
1	C	492	ARG
1	C	501	LEU

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Mol	Chain	Res	Type
1	C	505	LEU
1	C	506	LEU
1	C	509	LEU
1	C	516	GLU
1	C	541	ARG
2	D	544	VAL
2	D	557	LEU
2	D	563	VAL
2	D	569	GLU
2	D	575	LEU
2	D	583	ARG
2	D	601	PRO
2	D	603	VAL
2	D	604	LYS
2	D	609	LYS
2	D	611	LEU
2	D	618	LEU
2	D	620	HIS
2	D	625	LYS
2	D	630	THR
2	D	638	LYS
2	D	677	VAL
2	D	687	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	89	HIS
1	A	97	ASN
2	B	245	ASN
1	C	472	HIS
1	C	497	ASN
2	D	620	HIS
2	D	623	ASN
2	D	645	ASN
2	D	686	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	1142	1,4	50,50,50	1.57	10 (20%)	67,82,82	1.65	16 (23%)
4	OXY	A	1143	3	1,1,1	0.02	0	-		
4	OXY	D	1691	3	1,1,1	0.16	0	-		
4	OXY	B	1291	3	1,1,1	0.25	0	-		
3	HEM	B	1290	2,4	50,50,50	1.58	10 (20%)	67,82,82	1.83	20 (29%)
4	OXY	C	1543	3	1,1,1	0.43	0	-		
3	HEM	D	1690	2,4	50,50,50	1.47	10 (20%)	67,82,82	1.90	20 (29%)
3	HEM	C	1542	1,4	50,50,50	1.47	10 (20%)	67,82,82	1.39	12 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	1542	1,4	-	4/14/54/54	-
3	HEM	D	1690	2,4	-	1/14/54/54	-
3	HEM	A	1142	1,4	-	6/14/54/54	-
3	HEM	B	1290	2,4	-	2/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1290	HEM	FE-NC	4.52	2.10	1.95
3	C	1542	HEM	FE-NB	3.94	2.07	1.94
3	D	1690	HEM	FE-NC	3.67	2.07	1.95
3	A	1142	HEM	CAC-C3C	3.63	1.57	1.47
3	A	1142	HEM	FE-NA	3.47	2.06	1.95
3	D	1690	HEM	CAC-C3C	3.39	1.56	1.47
3	B	1290	HEM	CAC-C3C	3.27	1.56	1.47
3	D	1690	HEM	C2A-C3A	-3.16	1.30	1.38
3	C	1542	HEM	FE-NC	3.10	2.05	1.95
3	C	1542	HEM	CMD-C2D	3.00	1.56	1.50
3	D	1690	HEM	CMB-C2B	2.89	1.56	1.50
3	A	1142	HEM	CMB-C2B	2.89	1.56	1.50
3	A	1142	HEM	C2A-C3A	-2.88	1.31	1.38
3	A	1142	HEM	FE-NC	2.81	2.04	1.95
3	B	1290	HEM	CAB-C3B	2.78	1.54	1.47
3	C	1542	HEM	CAB-C3B	2.77	1.54	1.47
3	A	1142	HEM	CHC-C1C	2.71	1.43	1.38
3	B	1290	HEM	C1D-ND	2.69	1.44	1.38
3	D	1690	HEM	FE-NA	2.68	2.04	1.95
3	B	1290	HEM	C3C-C4C	2.65	1.50	1.46
3	B	1290	HEM	CAD-C3D	2.63	1.58	1.51
3	D	1690	HEM	CAB-C3B	2.62	1.54	1.47
3	A	1142	HEM	CMD-C2D	2.57	1.56	1.50
3	B	1290	HEM	C2A-C3A	-2.55	1.32	1.38
3	D	1690	HEM	O1A-CGA	2.51	1.30	1.22
3	C	1542	HEM	CAC-C3C	2.47	1.54	1.47
3	B	1290	HEM	FE-NA	2.43	2.03	1.95
3	A	1142	HEM	FE-ND	2.34	2.02	1.94
3	A	1142	HEM	CAB-C3B	2.33	1.53	1.47
3	B	1290	HEM	C3B-C2B	-2.28	1.32	1.37
3	D	1690	HEM	FE-NB	2.23	2.01	1.94
3	C	1542	HEM	CMB-C2B	2.21	1.55	1.50
3	C	1542	HEM	O1A-CGA	2.19	1.29	1.22
3	C	1542	HEM	O2D-CGD	-2.18	1.23	1.30
3	D	1690	HEM	CMA-C3A	2.10	1.55	1.50
3	A	1142	HEM	FE-NB	2.10	2.01	1.94
3	C	1542	HEM	FE-ND	2.07	2.01	1.94
3	B	1290	HEM	CMC-C2C	2.05	1.55	1.50
3	D	1690	HEM	C3C-C2C	-2.04	1.33	1.37
3	C	1542	HEM	C3D-C2D	-2.01	1.32	1.36

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1690	HEM	CMA-C3A-C4A	-4.59	118.44	125.42
3	B	1290	HEM	CMA-C3A-C4A	-4.32	118.83	125.42
3	D	1690	HEM	CMA-C3A-C2A	4.21	134.55	125.62
3	D	1690	HEM	CHC-C4B-NB	4.03	128.76	124.42
3	A	1142	HEM	CAA-C2A-C1A	-3.99	117.15	124.94
3	A	1142	HEM	CHA-C4D-ND	3.92	129.21	124.37
3	D	1690	HEM	CAD-CBD-CGD	3.85	123.86	113.67
3	D	1690	HEM	O1A-CGA-CBA	-3.84	110.92	123.09
3	B	1290	HEM	CAA-C2A-C3A	3.73	135.43	127.07
3	B	1290	HEM	CAD-C3D-C4D	-3.68	118.28	124.70
3	B	1290	HEM	CAA-C2A-C1A	-3.68	117.75	124.94
3	D	1690	HEM	CMD-C2D-C1D	-3.52	119.53	125.03
3	B	1290	HEM	O2A-CGA-CBA	3.48	125.01	114.00
3	C	1542	HEM	CHA-C4D-C3D	3.46	131.60	125.23
3	D	1690	HEM	CBA-CAA-C2A	-3.25	103.55	112.53
3	A	1142	HEM	C1A-CHA-C4D	-3.21	118.71	126.25
3	B	1290	HEM	C4C-C3C-C2C	3.08	109.49	106.81
3	D	1690	HEM	C1C-CHC-C4B	-3.01	119.63	126.02
3	A	1142	HEM	CAD-CBD-CGD	-2.95	105.84	113.67
3	C	1542	HEM	CBA-CAA-C2A	2.93	120.65	112.53
3	A	1142	HEM	C1A-C2A-C3A	2.84	111.26	106.87
3	A	1142	HEM	CHA-C1A-NA	2.83	128.99	123.86
3	D	1690	HEM	C3B-C2B-C1B	2.82	108.53	106.41
3	D	1690	HEM	CHB-C1B-NB	2.81	127.85	124.37
3	B	1290	HEM	CMA-C3A-C2A	2.81	131.59	125.62
3	C	1542	HEM	CBD-CAD-C3D	-2.81	104.76	112.53
3	B	1290	HEM	C1B-NB-C4B	-2.80	101.89	105.21
3	B	1290	HEM	O2D-CGD-O1D	-2.78	116.18	123.33
3	A	1142	HEM	CBD-CAD-C3D	-2.76	104.90	112.53
3	A	1142	HEM	CAA-CBA-CGA	-2.76	106.35	113.67
3	B	1290	HEM	CHD-C4C-NC	2.71	127.41	124.45
3	C	1542	HEM	C3D-C4D-ND	-2.70	107.21	110.17
3	A	1142	HEM	C2A-C1A-NA	-2.70	107.16	110.15
3	D	1690	HEM	CHA-C4D-C3D	2.70	130.20	125.23
3	C	1542	HEM	C1A-CHA-C4D	2.66	132.50	126.25
3	C	1542	HEM	CHA-C4D-ND	-2.63	121.11	124.37
3	C	1542	HEM	CMA-C3A-C2A	2.56	131.06	125.62
3	D	1690	HEM	C4C-C3C-C2C	2.55	109.03	106.81
3	C	1542	HEM	O1A-CGA-CBA	2.54	131.15	123.09
3	B	1290	HEM	CHB-C4A-NA	2.54	128.47	123.86
3	D	1690	HEM	CHA-C1A-C2A	2.54	130.86	125.30
3	C	1542	HEM	CHA-C1A-C2A	2.54	130.85	125.30
3	A	1142	HEM	CHD-C4C-C3C	2.45	129.34	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1290	HEM	C4A-C3A-C2A	2.41	109.58	106.82
3	B	1290	HEM	O2A-CGA-O1A	-2.40	117.15	123.33
3	C	1542	HEM	C4D-ND-C1D	2.38	108.03	105.21
3	D	1690	HEM	O2A-CGA-CBA	2.38	121.51	114.00
3	A	1142	HEM	C4C-CHD-C1D	2.37	131.06	126.02
3	B	1290	HEM	C3B-C4B-NB	2.36	111.17	109.47
3	A	1142	HEM	CHD-C4C-NC	-2.36	121.88	124.45
3	B	1290	HEM	CAD-C3D-C2D	2.34	132.25	127.87
3	D	1690	HEM	CAC-C3C-C4C	-2.29	119.36	124.82
3	A	1142	HEM	CBA-CAA-C2A	-2.27	106.26	112.53
3	D	1690	HEM	CMD-C2D-C3D	2.21	132.12	126.15
3	A	1142	HEM	O1D-CGD-CBD	-2.21	116.09	123.09
3	B	1290	HEM	C2B-C1B-NB	2.20	112.37	109.84
3	C	1542	HEM	CMA-C3A-C4A	-2.18	122.09	125.42
3	D	1690	HEM	CHA-C4D-ND	-2.17	121.68	124.37
3	B	1290	HEM	CAC-C3C-C4C	-2.17	119.63	124.82
3	D	1690	HEM	CHD-C4C-NC	-2.16	122.10	124.45
3	B	1290	HEM	CMC-C2C-C3C	2.16	133.66	128.43
3	D	1690	HEM	C2A-C1A-NA	-2.16	107.76	110.15
3	A	1142	HEM	CMA-C3A-C2A	2.14	130.16	125.62
3	C	1542	HEM	CHA-C1A-NA	-2.11	120.03	123.86
3	B	1290	HEM	C4A-CHB-C1B	-2.08	121.35	126.25
3	B	1290	HEM	C3C-C2C-C1C	-2.08	105.08	107.05
3	D	1690	HEM	CAA-C2A-C1A	-2.05	120.94	124.94
3	A	1142	HEM	CHD-C1D-C2D	2.04	128.25	125.03

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1142	HEM	C2B-C3B-CAB-CBB
3	A	1142	HEM	C4B-C3B-CAB-CBB
3	A	1142	HEM	CAD-CBD-CGD-O1D
3	D	1690	HEM	C3D-CAD-CBD-CGD
3	B	1290	HEM	CAD-CBD-CGD-O2D
3	C	1542	HEM	CAD-CBD-CGD-O1D
3	B	1290	HEM	CAD-CBD-CGD-O1D
3	C	1542	HEM	CAD-CBD-CGD-O2D
3	A	1142	HEM	CAA-CBA-CGA-O2A
3	A	1142	HEM	CAD-CBD-CGD-O2D
3	A	1142	HEM	CAA-CBA-CGA-O1A
3	C	1542	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	C	1542	HEM	C2B-C3B-CAB-CBB

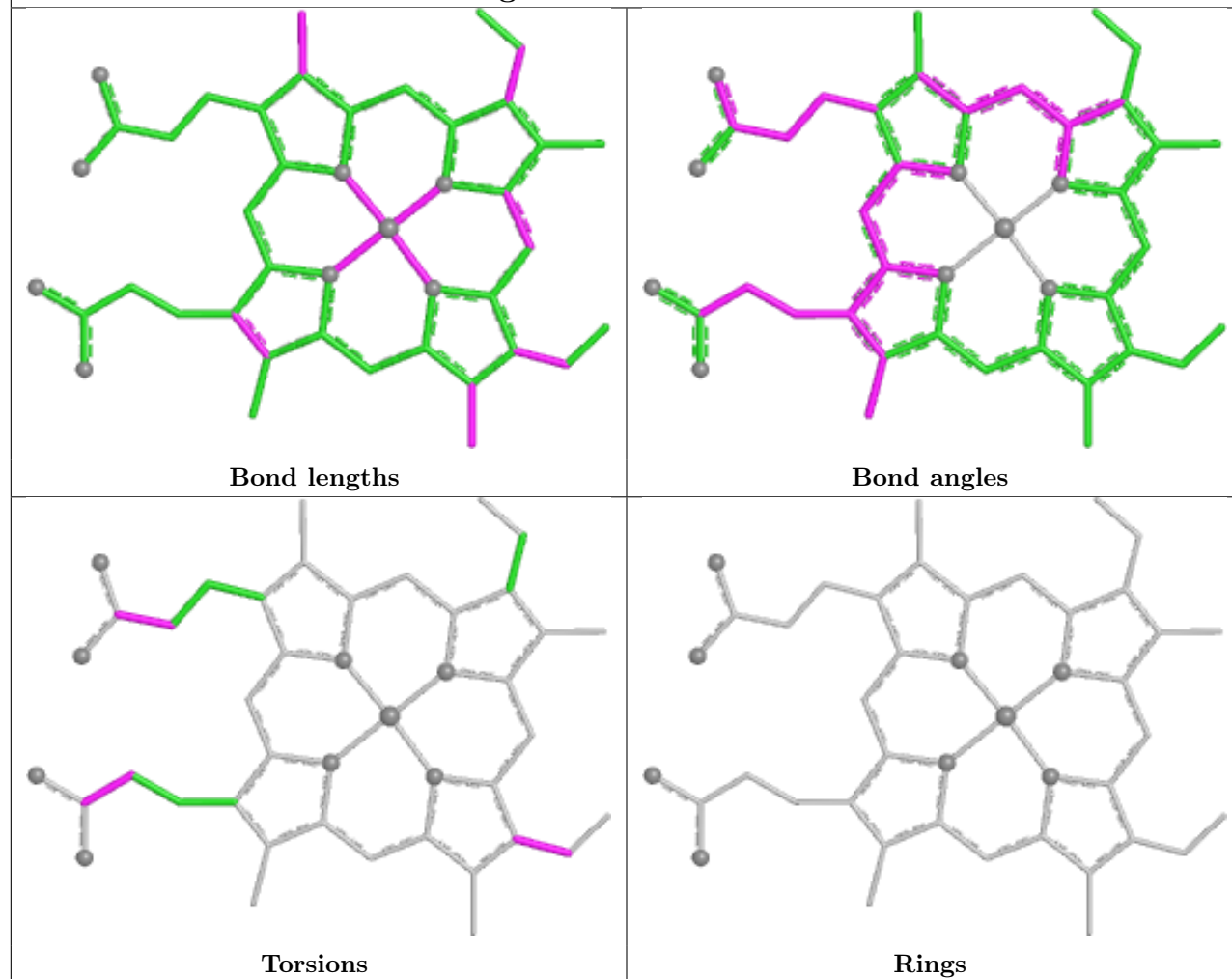
There are no ring outliers.

5 monomers are involved in 18 short contacts:

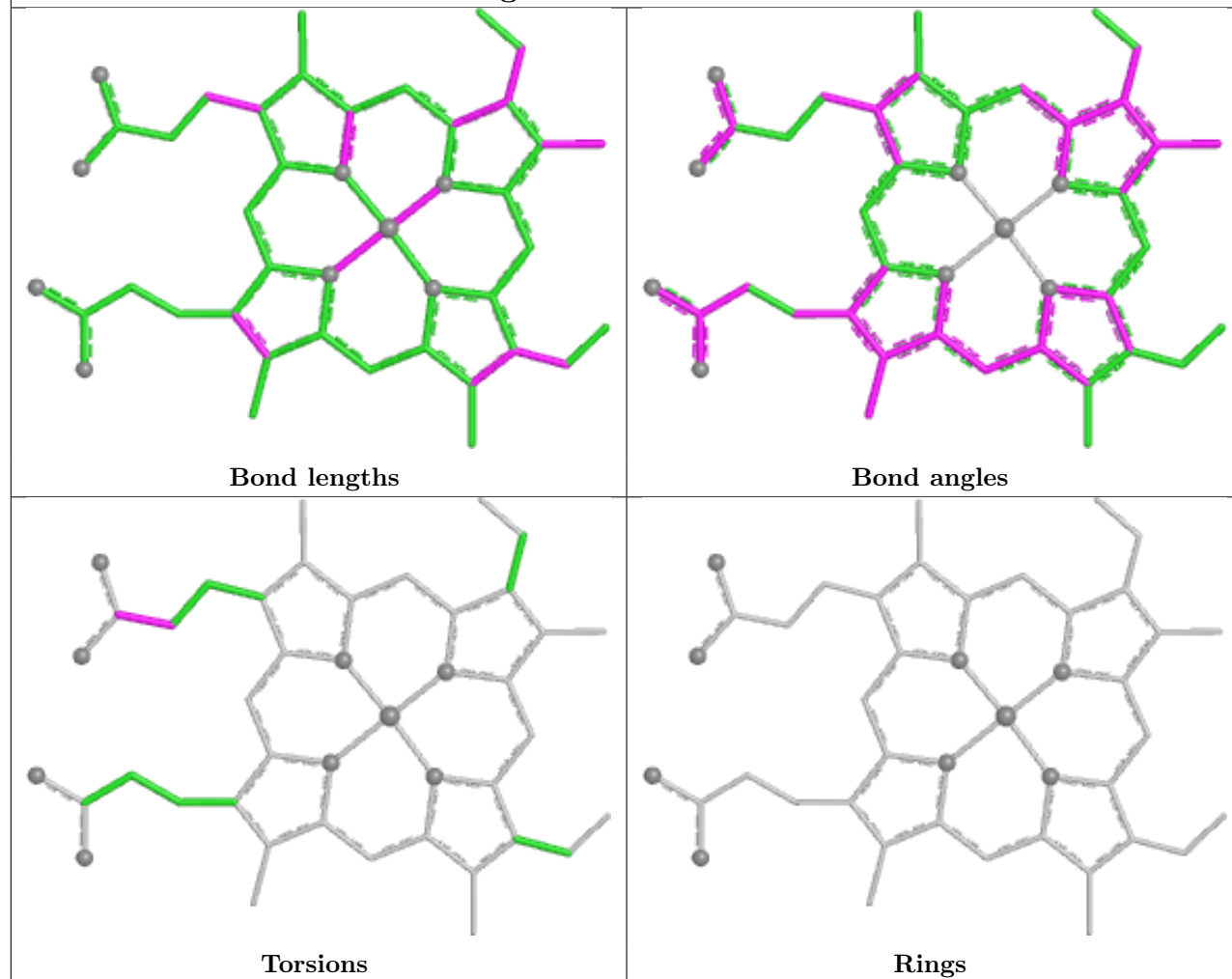
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1142	HEM	3	0
4	D	1691	OXY	2	0
4	B	1291	OXY	2	0
3	B	1290	HEM	1	0
3	D	1690	HEM	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

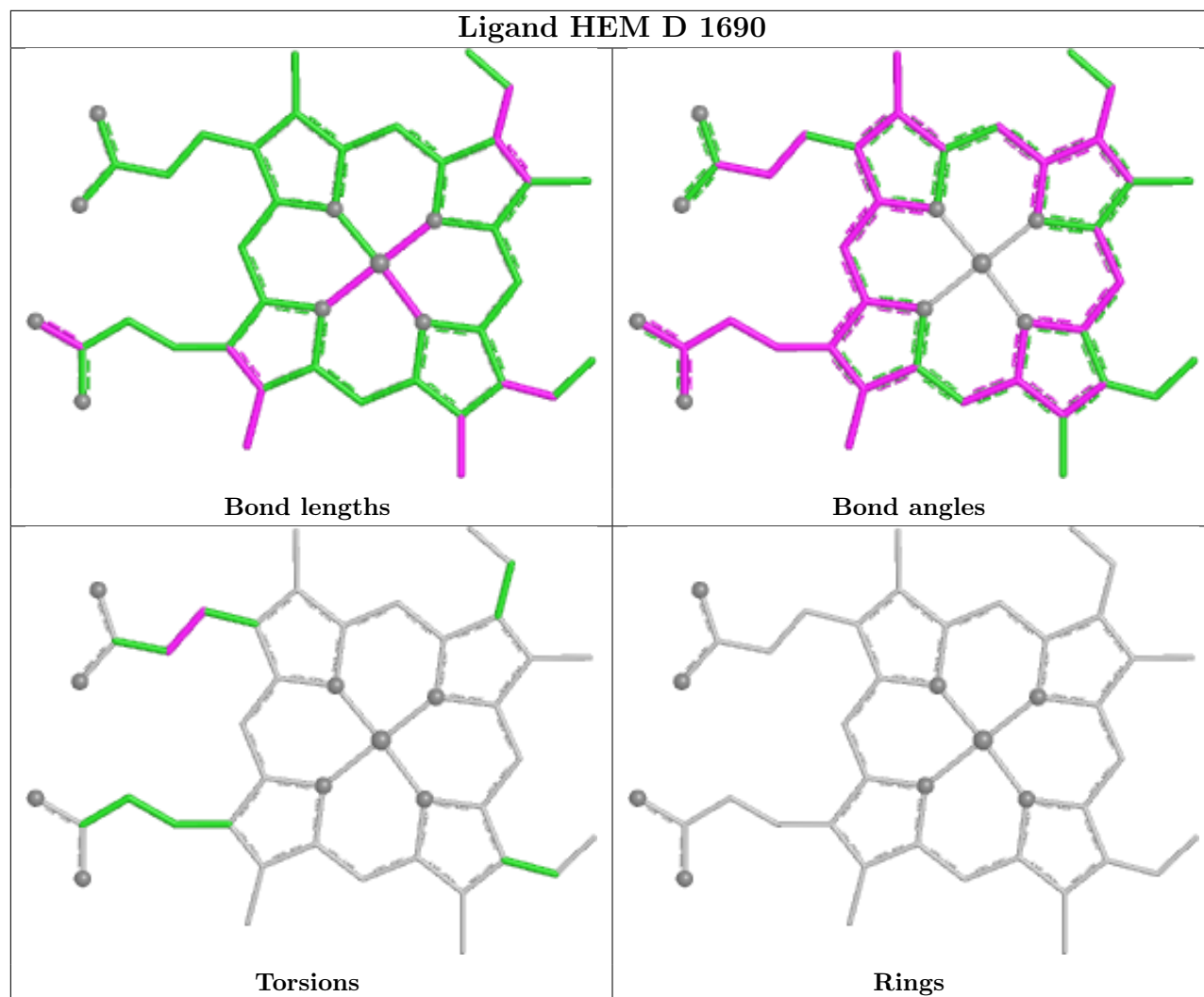
Ligand HEM A 1142

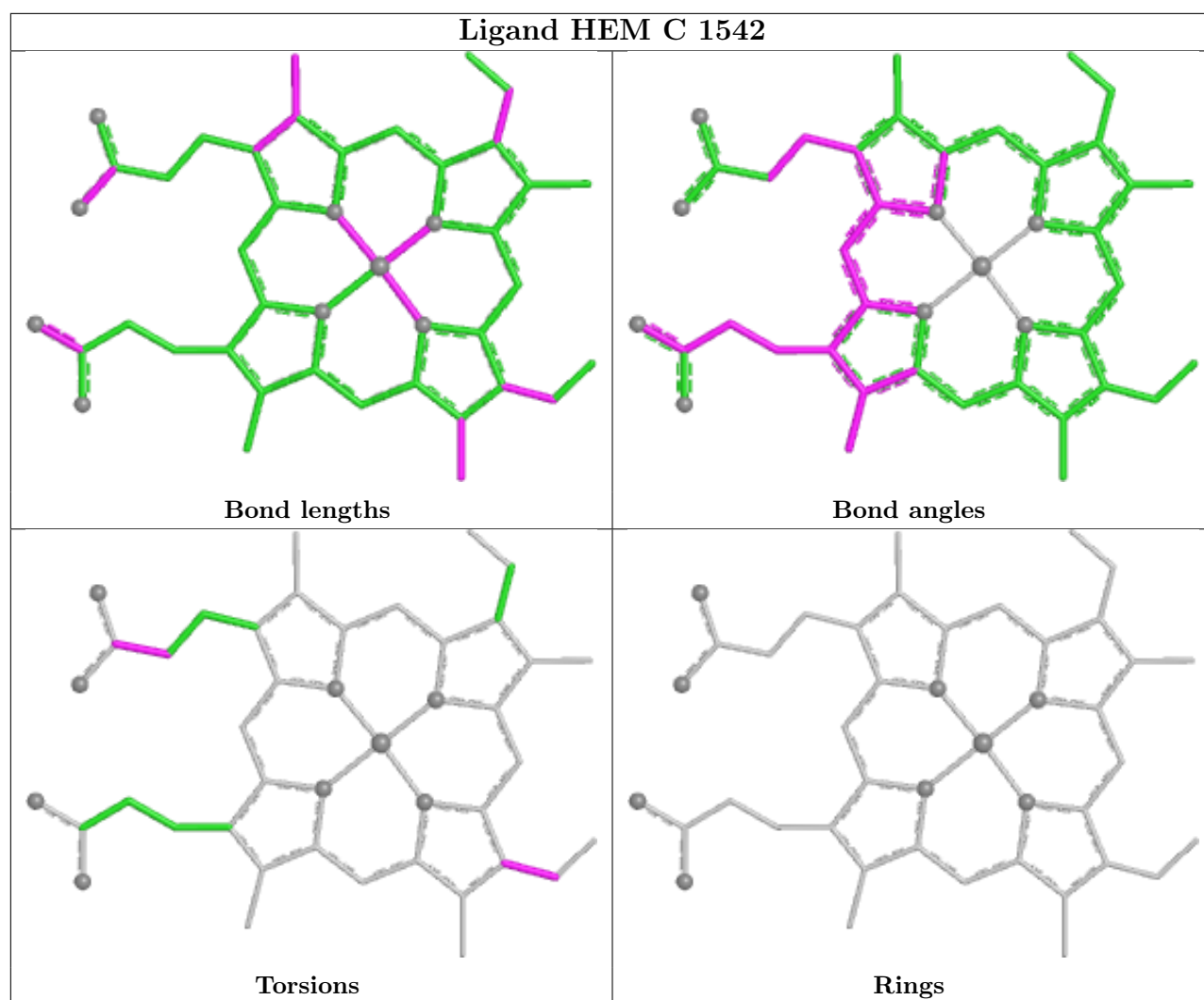


Ligand HEM B 1290



Ligand HEM D 1690





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/141 (100%)	-0.67	0 100 100	17, 24, 35, 44	0
1	C	141/141 (100%)	-0.54	0 100 100	14, 27, 37, 46	0
2	B	146/146 (100%)	-0.62	0 100 100	15, 23, 40, 54	0
2	D	146/146 (100%)	-0.42	0 100 100	16, 28, 42, 55	0
All	All	574/574 (100%)	-0.56	0 100 100	14, 26, 40, 55	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OXY	A	1143	2/2	0.91	0.09	27,27,27,33	0
4	OXY	C	1543	2/2	0.95	0.06	25,25,25,30	0
3	HEM	A	1142	43/43	0.96	0.06	23,27,36,44	0
4	OXY	B	1291	2/2	0.96	0.12	19,19,19,21	2

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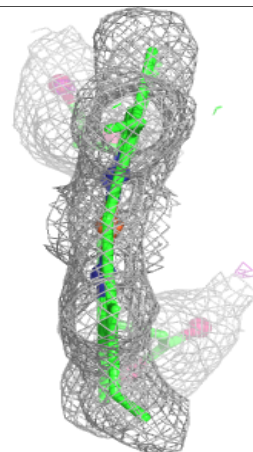
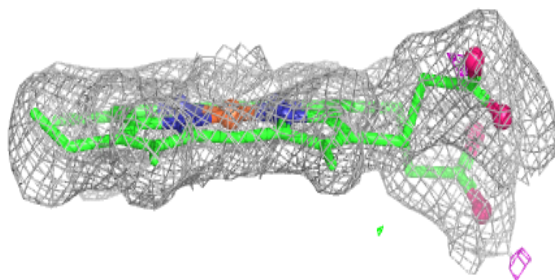
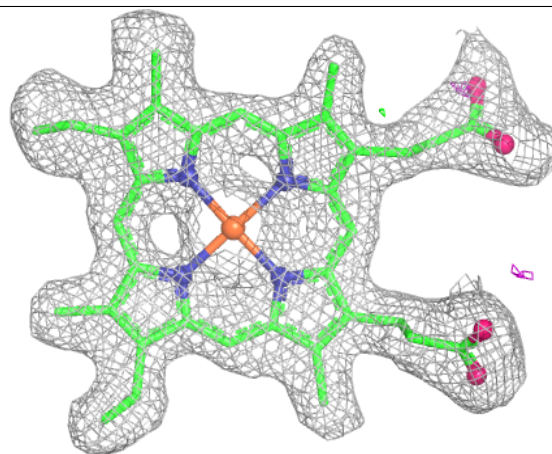
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	D	1690	43/43	0.96	0.06	25,28,40,42	0
4	OXY	D	1691	2/2	0.96	0.12	30,30,30,36	0
3	HEM	C	1542	43/43	0.97	0.06	17,22,34,40	0
3	HEM	B	1290	43/43	0.98	0.05	13,18,25,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

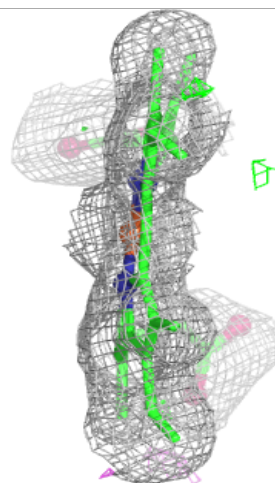
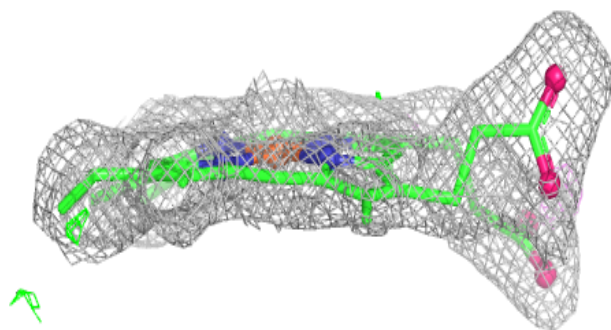
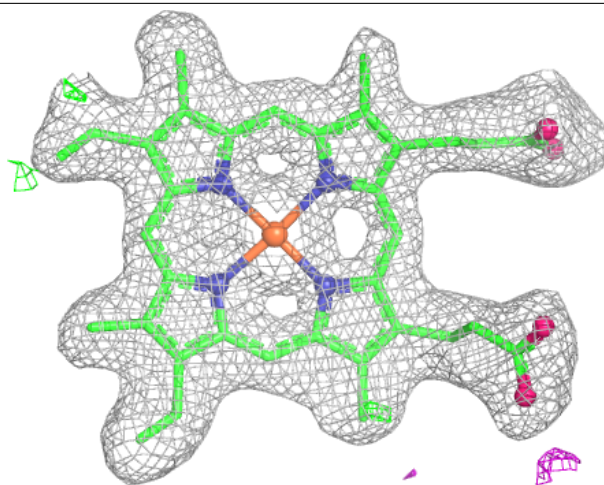
Electron density around HEM A 1142:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



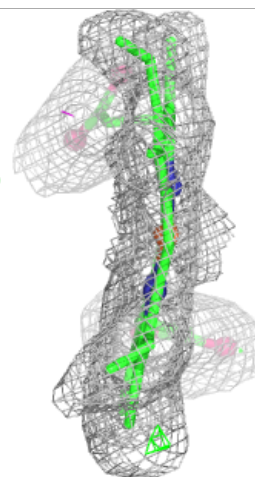
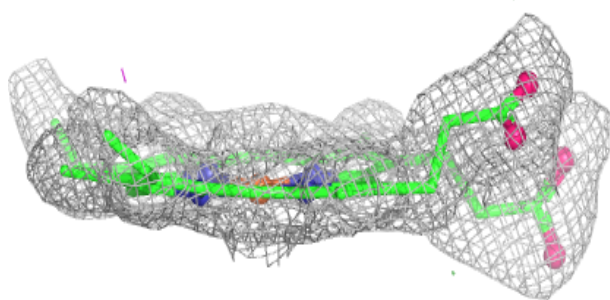
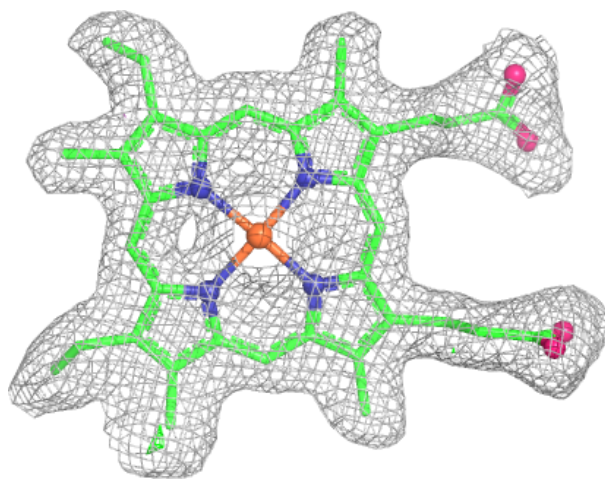
Electron density around HEM D 1690:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



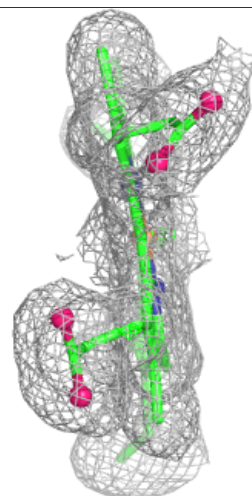
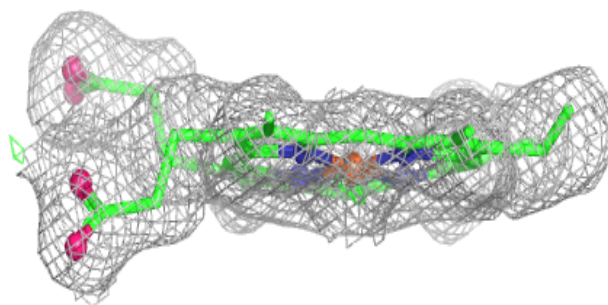
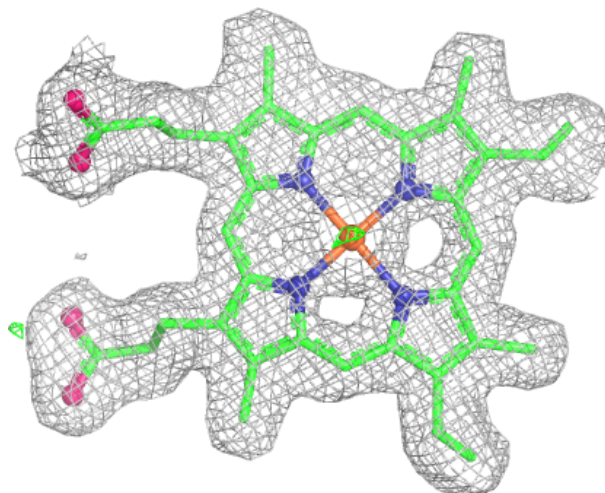
Electron density around HEM C 1542:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 1290:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.